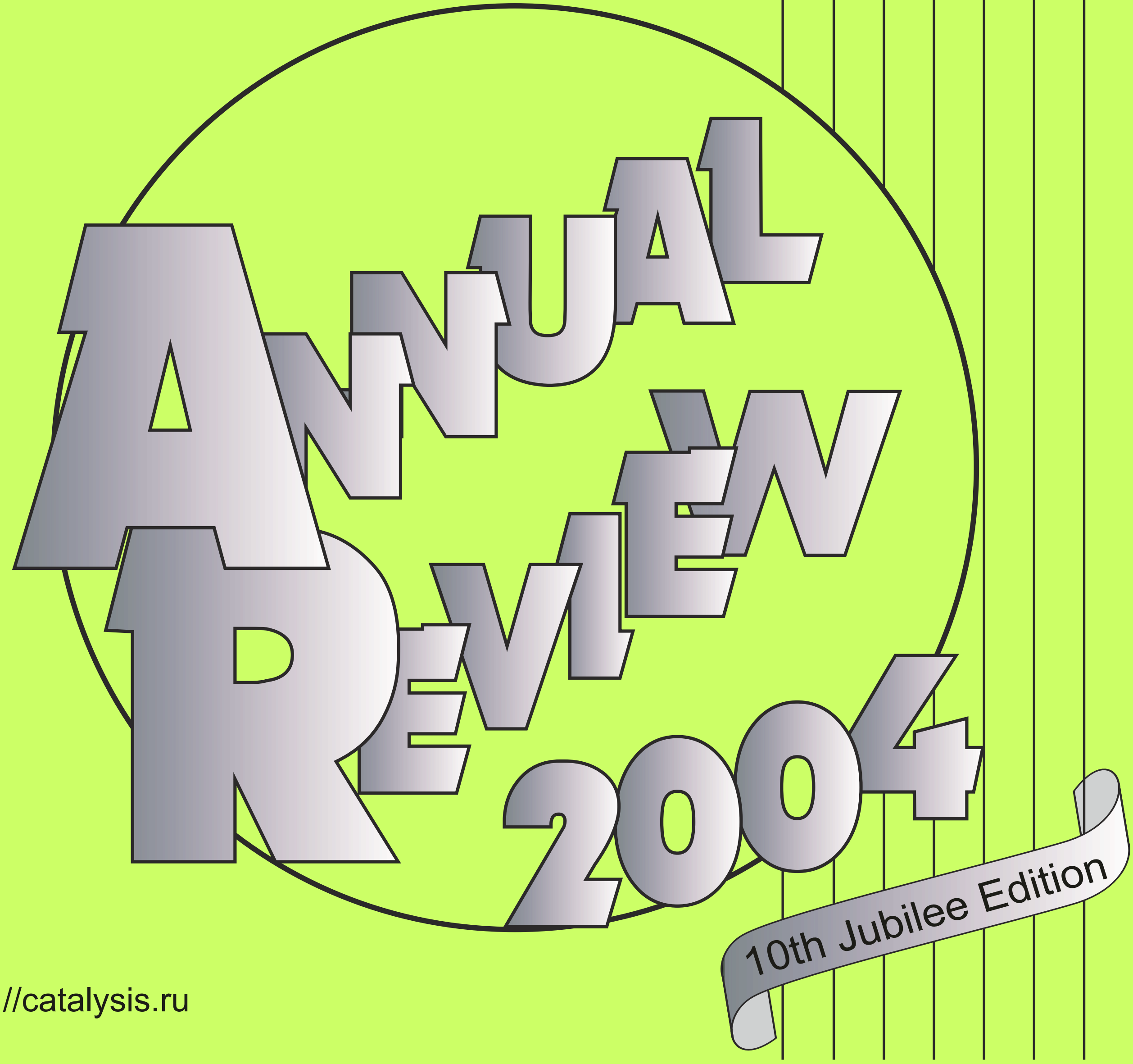
BORESKOV INSTITUTE OF CATALYSIS

SIBERIAN BRANCH OF RUSSIAN ACADEMY OF SCIENCES

45 ANNIVERSARY

ANNUAL REVIEW 2004

10th Jubilee Edition



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of Activities in Fundamental Areas
2003

BOREKOV INSTITUTE OF CATALYSIS
SIBERIAN BRANCH OF RUSSIAN ACADEMY OF SCIENCES

Novosibirsk

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Dear Colleagues,

This issue of the Annual Review of the Boreskov Institute of Catalysis in the main fields of its academic and R&D activities covers the year 2003 and reflects already the ten-year experience of the Institute in publishing such reviews.

The Boreskov Institute of Catalysis, or BIC, is well known to experts in both academic and industrial catalysis not only in Russia and NIS, but also in many western and oriental countries. Since the sixties of the 20th century it remains the largest Russian chemical research institution in the Asian part of Russia and has many deep and stable traditions in providing basic and applied research in nearly all fields of catalysis. The interests of BIC spread from the sophisticated areas of purely academic research to the real applied problems, including development of commercial catalysts and catalytic technologies.

The current features of BIC reflect Russia entering into the market economy. BIC belongs to the Siberian branch of the Russian Academy of Sciences. However, according to new realities of Russia, a lot deal of activity of BIC is now devoted not only to basic research, but also to numerous industrially oriented topics. The intensity and quality of the research and engineering activity at the Institute became at new period of the Russia’ history even higher as before. Fortunately, the Institute gained in research in catalysis fundamentals, thus continuing the old traditions originated from the beginning of the Institute due to a very powerful impulse of its creator and first director Academician Georgii K. Boreskov, as well as the master ideas of the second director Academician Kirill I. Zamaraev. Hope, the readers will feel that themselves, when comparing the materials of this and previous issues of the Annual Review.

The year 2003 was very important for life of the Russian science as well as that of BIC in many aspects. First of all, for the Institute, this year was the year of the 45th anniversary of BIC. Also, after a long period of stagnation of the Russian authority’s attitude to science, at the year 2003 the first call for the really large governmental grants for R&D innovations took place. BIC participated in the strong competition for such grants and won the largest in the history of new Russia grant to transfer the newly developed generation of catalysts and catalytic technologies to the Russian oil-refineries. So, starting from this moment, the main R&D priority of BIC for the next three years will be, indeed, successful accomplishing the work directed to the area of the

Russian oil refining. Starting from the end of 2003, the second highly important priority of BIC appeared to be the collaboration with another Russian industrial partner in the field of the development of hydrogen generators for modern fuel cells. Thus, the reestablishing strategic collaboration with the Russian industries undoubtedly is now a new and very important feature for the scientific activity of the Boreskov Institute, as well as for many academic institutes of RAS.

Since 1998 the Institute is operating in the status of the Key Russian institution and federal coordinator in the field of catalysis and catalytic technologies, i.e. in the very high federal status, the same as the Institute had in the former USSR. From that year the Institute succeeded also in reestablishing the National Russian R&D program in new generation of catalysts and catalytic technologies sponsored by the Ministry of Industry, Science and Technologies of the Russian Federation.

Since 1998 the Institute has been united with some other R&D chemical institutions of the Siberian Branch of the Russian Academy of Sciences in the frame of a new R&D association, which was called the United Institute of Catalysis (UIC). According to the UIC bylaw, the director of the Boreskov Institute of Catalysis is simultaneously the general director of the UIC. In 2003, the United Institute of Catalysis included the Boreskov Institute of Catalysis with its Omsk and St. Petersburg Divisions, the Research and Engineering Institute for Technical Carbon in Omsk as well as Scientific-Engineering Center “Zeosit” in Novosibirsk and Volgograd Scientific-Engineering Center on the Volga River. The facilities of the UIC include now three powerful semi-industrial plants capable of providing manufacturing of the first industrial batches of various catalysts and specialty chemicals. At the end of 2003, UIC has been reorganized a little. The Omsk Division of BIC and the Institute of Technical Carbon have merged together into new UIC’s Institute of the Trends in Hydrocarbon Processing. Thus, BIC together with UIC create now one of the most powerful Russian specialized R&D organizations in the industry-oriented chemistry. Indeed, current management of the Institute is recognizing well all the existing problems and trying to take care in the maintenance of high activity and productivity of R&D of BIC and UIC in both fundamental and applied areas as the goal of the highest priority.

Hope this Anniversary issue of the Annual Review of the Boreskov Institute of Catalysis is exhibiting many sides of the current Institute’s capacity in basic research on catalysis, catalysts and catalytic technologies. As to the activity of the Institute in the applied areas, which is now much more active than in the past, we publish special leaflets or are inviting to visit the Institute’s website.

Valentin N. Parmon

BORESKOV INSTITUTE OF CATALYSIS
OF THE SIBERIAN BRANCH
OF THE RUSSIAN ACADEMY OF SCIENCES

The Boreskov Institute of Catalysis of the Siberian Branch of the Russian Academy of Sciences (BIC) still remains the largest specialized institute working in the field of catalysis not only at the territory of Asian part of Russia, but in the world too. It is the only institution in the country fully specialized on the problems of catalysis and encompasses all its aspects from fundamental and theoretical to industrial mastering of new catalysts.

The Institute was founded in 1958. Initiator of the Institute and its permanent director up to 1984 was Academician Georgii K. Boreskov (1907-1984), an eminent scientist with international recognition, an outstanding physical chemist and chemical technologist. In 1992 the Institute of Catalysis was named after Academician G.K. Boreskov.

In 1976 Professor Kirill I. Zamaraev has been invited by Academician G.K. Boreskov to join the Institute of Catalysis as a Deputy Director. Kirill Ilyich has come to Novosibirsk at early 1977 together with a large team of young chemical physicists, thus largely widening the studies of elementary catalytic reactions on molecular-atomic level through application of modern physical and kinetic instrumental methods of investigation.

In 1984 Professor Zamaraev became the Director of the Institute of Catalysis, and since that time he was the real leader of all research and development activity of this huge (up to 1000 people in staff) Institute. K.I. Zamaraev, the former President of the International Union of Pure and Applied Chemistry, Foreign Fellow of the Indian National Science Academy and of the Korean Academy of Science and Technology, holder of the Silver Medal of the Royal Chemical Society of Great Britain as a centenary lecture, has passed away in the prime of his brilliant scientific career on 26 June 1996.

In 1995 Professor Valentin N. Parmon, prominent specialist in the field of catalysis, chemical kinetics and photocatalysis, headed the third generation of the directorate of the Institute.

Since 1998 the Institute has been united with some other R&D chemical institutions of the Siberian Branch of the Russian Academy of Sciences in the frame of a new R&D association: the United Institute of Catalysis headed by the director of the Boreskov Institute of Catalysis. Now the United Institute of Catalysis (UOC) includes the Boreskov Institute of Catalysis with its Omsk and St. Petersburg Divisions, the Research and Engineering Institute for Technical Carbon in Omsk as well as Scientific-Engineering Center “Zeosit” in Novosibirsk and Volgograd Scientific-Engineering Center on the Volga River.

STRUCTURE OF THE INSTITUTE

The Institute of Catalysis with its Omsk and St. Petersburg Divisions currently has 1000 employees including researchers and their co-workers, of these 2 Members of the RAS, 4 Corresponding Members of the RAS, about 60 Professors, more than 200 have a Ph.D. degree, about 50 Ph.D. students, personnel of Service, Managing, Engineering and Pilot Departments to support and promote R&D activities. The Institute presents the unique society of qualified specialists in broad spectra of catalysts problems, able to solve any questions related to phenomena of catalysis, from theoretical problems like quantum-chemical calculations up to designing of industrial catalysts and processes.

The structure of the Institute incorporates 7 Scientific-Research Departments, Department of Applied Catalysis, Center for Catalyst Characterization and Testing, and Information Center. The structure of the Institute includes also scientific-supportive units, manufacturing facilities, administration and services.

The Center for Catalyst Characterization and Testing has a bank of catalyst samples, supports and adsorbents, a set of State Standard Samples to calibrate and certify instruments for measurements of specific surface areas of various dispersed and porous materials.

The main directions of its activity are:

- Complex investigation and characterization of the catalysts by a set of modern physicochemical methods.
- Joint scientific projects with foreign firms and organizations on studying certain catalytic processes and catalysts for the purpose of their improvement.
- Development of modern standard experimental methods and equipment for catalyst studies and tests. Design of catalysts and materials with certificated properties.

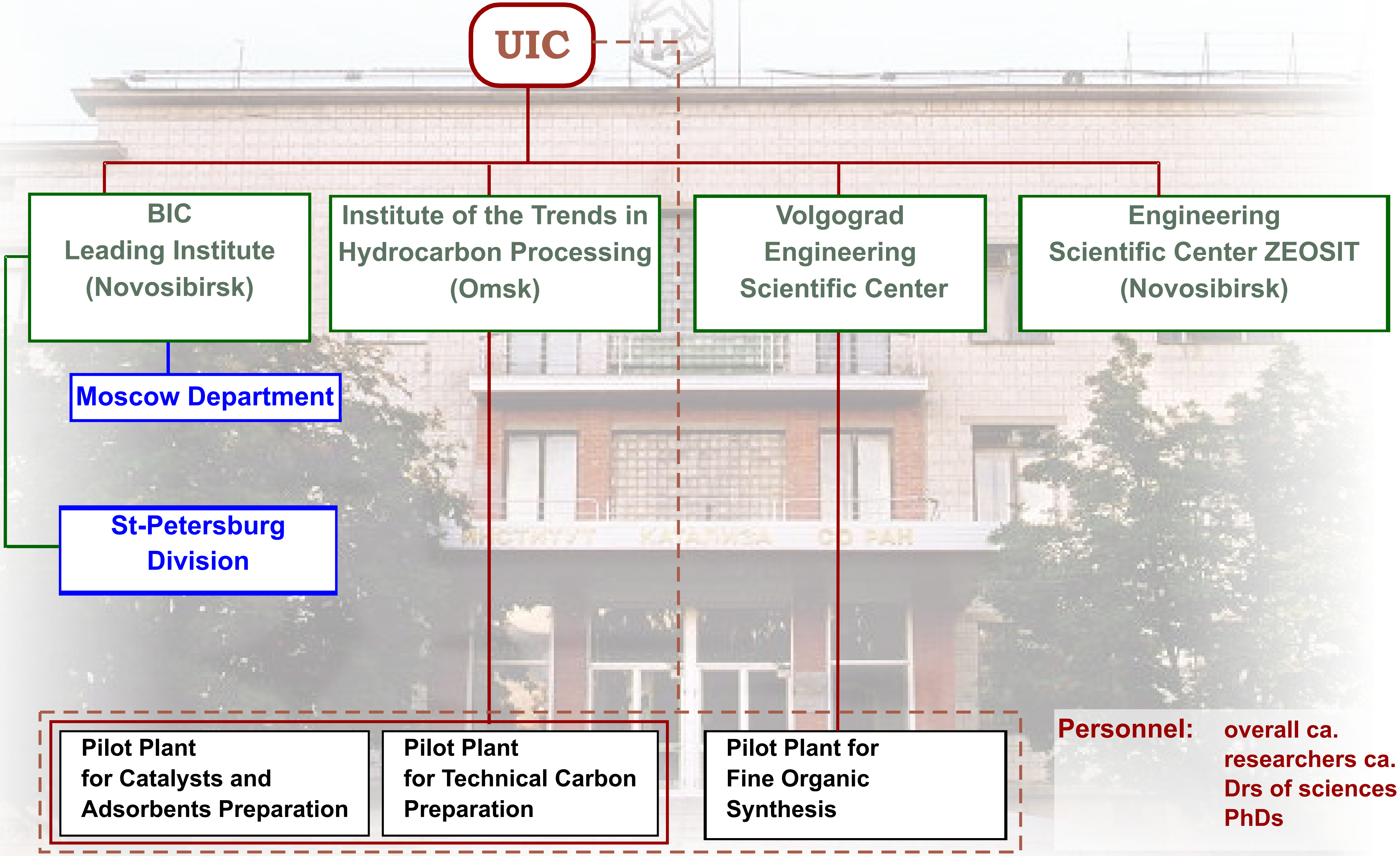
In its work Center bases on high potential of the Institute, its fundamental and applied studies in all fields of catalysis, its outdated instrumentation and methods for catalytic systems studying.

The Information Center of the Institute comprises the Library of Scientific Literature and the Group of mathematical and program support. It has developed the information system 'Catalysis', which includes the updated data bases, such as the bibliography and the actual state of the art, related to research and applied works in the field of catalysts, commercial catalysis and catalytic processes developed in foreign countries and countries of the former USSR. The Centre can connect with remote databases through Internet and offers information on clients request.

Department of Applied Catalysis with a complex bench of adoption and testing of processes and catalysts provides commercialization of new developments in shortest time.

UNITED INSTITUTE OF CATALYSIS (UIC)

Founded in 1997



UIC

BIC
Leading Institute
(Novosibirsk)

Moscow Department

St-Petersburg
Division

Institute of the Trends in
Hydrocarbon Processing
(Omsk)

Volgograd
Engineering
Scientific Center

Engineering
Scientific Center ZEOSIT
(Novosibirsk)

Pilot Plant
for Catalysts and
Adsorbents Preparation

Pilot Plant
for Technical Carbon
Preparation

Pilot Plant for
Fine Organic
Synthesis

Personnel:

overall ca.	1200
researchers ca.	450
Drs of sciences	70
PhDs	230

STRUCTURE OF THE INSTITUTE

Directorate:
V.A. Sobyanin, R.A. Buyanov, V.N. Parmon,
A.S. Noskov, B.I. Ermakov, O.N. Martyanov,
S.P. Kildyashev, S.E. Glaznev, B.S. Bal'zhinimaev,
I.A. Kamolkin, V.I. Bukhtiyarov

DIRECTOR

Directorate

Scientific Council

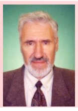
Research Departments

ИК
СО РАН

DEPARTMENT OF PHYSICOCHEMICAL METHODS FOR CATALYST INVESTIGATION
Head: Prof. Dimitrii I. Kochubey

DEPARTMENT OF NONTRADITIONAL CATALYTIC PROCESSES AND TECHNOLOGIES
Head: Acad. Valentin N. Parmon

DEPARTMENT OF HETEROGENEOUS CATALYSIS
Head: Prof. Vladimir A. Sobyanin



DEPARTMENT OF HOMOGENEOUS AND COORDINATION CATALYSIS
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DEPARTMENT OF EXPLORATORY AND APPLIED INVESTIGATIONS
Center for Catalyst Characterization and Testing
Head: Prof. Bair S. Bal'zhinimaev

DEPARTMENT OF CATALYTIC PROCESS ENGINEERING
Head: Prof. Alexander S. Noskov

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DEPARTMENT OF APPLIED CATALYSIS
Head: Dr. Il'ya A. Zolotarskii

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Administration and Services

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Laboratory of Adsorption
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Laboratory of Analytical Chemistry
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Laboratory of Spectral Methods
Head: Prof. Dimitrii I. Kochubey

Laboratory of Quantum Chemistry
Head: Dr. Igor L. Zilberberg

Surface Science Laboratory
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Head: Dr. Aleksey N. Salanov

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Group of Low Temperature Catalysis by Metals
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Group of Solid- State NMR Spectroscopy
Head: Prof. Olga B. Lapina

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Group of Aerosol Nucleation

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Group of Metal Complex Catalysis

Head: Dr. Nina I. Kuznetsova

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Group of Metallorganic Catalysts

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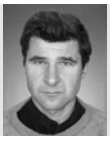
Head: Prof. Eugenii A. Paukshtis

Group of Catalysts Preparation
Head: Vasilii Yu. Kruglyakov

Group of Catalysts Testing
Head: Aleksandr S. Bobrin



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PROF. VALERII K. DUPLYAKIN

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Laboratory of Deep Petroleum Refining
Head: Prof. Valerii K. Duplyakin

Laboratory of Catalytic Methods for Atmosphere Protection
Head: Prof. Pavel G. Tsyrulnikov

Laboratory of Catalysis by Supported Metals
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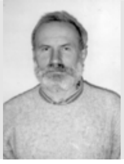
Head: Dr. Vladimir P. Doronin

SUBDIVISION OF PHYSICOCHEMICAL METHODS OF INVESTIGATION

Group of Adsorption
Head: Dr. Vladimir A. Drozdov



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Analytical Group
Head: Tatiana V. Kireeva

Group of X-Ray and Electron Microscopy Technique

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HEAD: KONSTANTIN V. KOLMOGOROV

ST. PETERSBURG DIVISION
OF THE BORESKOV INSTITUTE OF CATALYSIS

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PROF. SERGEY S. IVANCHEV

VICE-DIRECTOR DR. VALERY P. TULMANKOV

Laboratory of Micellar Catalysis, Emulsion Polymerization and Processes for Obtaining Polymeric Composites
Head: Prof. Valery N. Pavlyuchenko

Laboratory of Novel Catalytic Systems for Olefin Polymerization and Copolymerization
Head: Prof. Sergey S. Ivanchev

SCHOOLS OF THE BORESKOV INSTITUTE OF CATALYSIS

The Boreskov Institute of Catalysis has numerous and deep traditions and continues intensive fundamental and applied investigations. It possesses an actively and fruitfully working school of specialists in catalysis.

Many works by the school of **Acad. Georgii K. Boreskov** in the field of deep and partial oxidation processes are well known in our country and far from its frontiers.

The principal importance has the concept of chemical nature of phenomenon the decisive role in which belongs to the intermediate chemical interaction between the reagents and catalysts. The fundamentals of the theory of heterogeneous oxidative catalysis are:

— The key importance of the energy of reagent bonding to the catalyst for the rate and rote of oxidation reactions;

— The influence of cation nearest environment on catalytic properties;

— A viewpoint on reaction medium and catalyst as an indivisible system;

— An idea of stepwise and concerted mechanisms of redox reactions.

Under the guidance of **Prof. Mikhail G. Slin'ko** in 60-70th years a school raised famous not only in Russia, but abroad as well.

M.G. Slin'ko developed a method of mathematical modeling of catalytic reactors and processes, based on hierarchical principle. This method was developed for multi-phase processes and reactors with fixed and fluidized beds.

Design of real industrial catalysts with optimum strength, pore structure; providing their reproducibility on a large scale are the necessary elements of all aspects in the field of applied catalysis. **Prof. Vera A. Dzis'ko** contributed significantly to the development of methods of preparation and studying the regularities of oxide catalysts formation.

The revealed correlation of preparation conditions and physico-chemical properties of oxide systems allowed to formulate the criteria to control phase composition, surface area, stability, and acid-base properties, that appeared to be the basis for creation of a number of industrial catalysts and carriers.

At the end of the 60s big progress was in the field of homogeneous catalysis and catalysis by transition metal complexes. Of essential importance in this field not only for our country were the works by **Prof. Yurii I. Yermakov**.

Yu.I. Yermakov formulated the conception of the surface metal-organic compounds as active sites precursors for the supported catalysts. It served as a basis for the new approach in catalysis – application of principles used in homogeneous catalysis to study fundamental problems of heterogeneous catalysis. Methods for purposeful synthesis of supported catalysts of desired composition and dispersity have been developed.

In the 1977-1978 a big team of chemical physicists of the younger generation headed by **Acad. Kirill I. Zamaraev** came from Moscow. The flow of these specialists significantly enlivened the atomic-molecular studies of catalytic reaction mechanisms and catalytic properties of heterogeneous catalysis by physicochemical methods.

The school by K.I. Zamaraev contributed much to:

— Development of theory of electron tunneling in condensed media;

— Coordination chemistry of metal-complexes solutions;

— Step-wise description of homogeneous catalytic reactions;

— The works in photochemistry, photocatalysis and solar-to-chemical energy conversion.

The main principle of these works is the complex application of modern physico-chemical technique to mechanistic studies of heterogeneous and homogeneous reactions, studies of the structure and the active sites at the molecular level, search of new nontraditional directions in catalysis.

In 1999 the teams headed by Prof. Roman A. Buyanov, Prof. Vladimir A. Likholobov, Acad. Valentin N. Parmon, Prof. Georgii M. Zhidomirov won the competitive Program "Leading Scientific Schools" supported by RFBR.

Prof. Roman A. Buyanov developed the home school of fundamentals for catalyst preparation and technology**.**

The main research areas covered are:

— Design and application of new methods to increase solid phases activity at catalysts preparation and to control their activity and selectivity;

— Study of catalysts deactivation and carbon-mineral compositions formation;

— Development of the theory of non-branched radical chain reactions in the absence of oxygen (pyrolysis);

— Design of industrial catalysts.

The works by school of **Prof. Vladimir A. Likholobov** initiated development of methodological and fundamental approaches to the synthesis of effective homogeneous and heterogeneous catalysts for organic synthesis.

The main conceptions of this school are:

— Molecular design of catalytic compositions on all hierarchical levels;

— "Assembly" of active centers of metal complex catalysts;

— Synthesis of porous supports with desired texture and surface properties.

The works of school by **Acad**. **Valentin N. Parmon** relate to:

— Design and study of novel and nontraditional catalytic processes, first of all, photocatalytic and thermochemical methods for the direct conversion of solar energy and ionizing radiation energy;

— Development of an original approaches to description of catalytic processes by methods of nonequilibrium thermodynamics;

— Study of a possible impact of photocatalysis over the troposphere aerosols on the global chemistry of the Earth atmosphere.

The school of **Prof. Georgii M. Zhidomirov** develops the quantum-chemical direction in theoretical spectroscopy and molecular theory of catalysis:

The methodological basis for molecular (cluster) modeling of catalytic systems is formulated, the cluster approximation is widely used to calculation of electronic structure and reactivity of active sites on zeolites and oxide catalysts.

R&D ACTIVITY OF THE INSTITUTE

Fundamental catalysis

- Determination of general physico-chemical regularities of catalysis
- Development of scientific basis for molecular design of substances and materials
- Development of the theoretic basis for realization of catalytic processes.

Applied catalysis

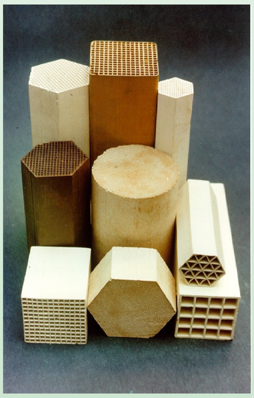
- Design of highly efficient catalysts of new generation for the production of key chemicals and oil processing
- Design of catalytic compositions and technologies for innovative application areas
- Development of innovative catalysts and catalytic technologies manufacturing complex chemicals and polymers with preconceivable properties
- Design of sorbents, catalysts and technologies for detoxication of hazardous technogenous wastes.

New catalytic technologies owned by BIC

- A family of new unsteady-state technologies in catalysis:
  - — «Reverse-process»
  - — Partial oxidation over unsteady-state catalysts
- A family of technologies based on combustion in a fluidized catalyst bed «Catalytic Heat Generators»
- Processing of oil, natural gas, and coal
- Large-scale inorganic synthesis
- Catalytic technologies for carbon-carbonaceous composites production

- Catalytic technologies for energy production
- Catalytic technologies for environmental protection
- Production of food, medicines, and biopreparations
- Purification of hydrocarbon-containing gases from H_2S *via* its partial oxidation to sulfur
- Processing of sulfur-containing organics
- Partial oxidation of organics with bounded oxygen
- Zeolite-based processes (zeoforming, condensation, nitration)
- Catalytic partial oxidation of aromatics under unsteady-state conditions
- Oxidation of methanol in an adiabatic catalyst bed to produce formaldehyde
- Direct oxidation of methanol to formic acid
- Direct gas-phase oxidation of β-picoline to nicotinic acid

Catalytic Processes from Molecular Level to Industrial Plants



2003 BIMF process - production of high-quality motor fuels, Russia

2002 Selective water sorbents, Russia

2001 Reforming catalysts, Russia

BCS , Estonia, 2001

2000 New technology of loading the reactors with catalysts, Russia

1999 Catalyst for hydropurification of terephthalic acid

Developed in cooperation with Samsung Chemicals, Korea, 2000

1998 One-step technology for production of nicotinic acid, Russia

Degussa, Germany, 2000

1997 Non-platinum catalyst for production of nitric acid, Russia

1996 ALPHOX technology (benzene + [N_2O] → phenol)

Jointly designed with SOLUTIA, USA, 1996

1995 Catalyst for FCC (oil cracking), Russia

1993 Carbonaceous material SIBUNIT, Russia

Sibunit for phosgene synthesis, DuPont, 1994, USA

1992 ZEOFORMING process for synthesis of gasoline, Russia

Lurgi, Germany, 1994

1988 Catalysts for polypropylene polymerization, USSR

DSM, the Netherlands, 1995

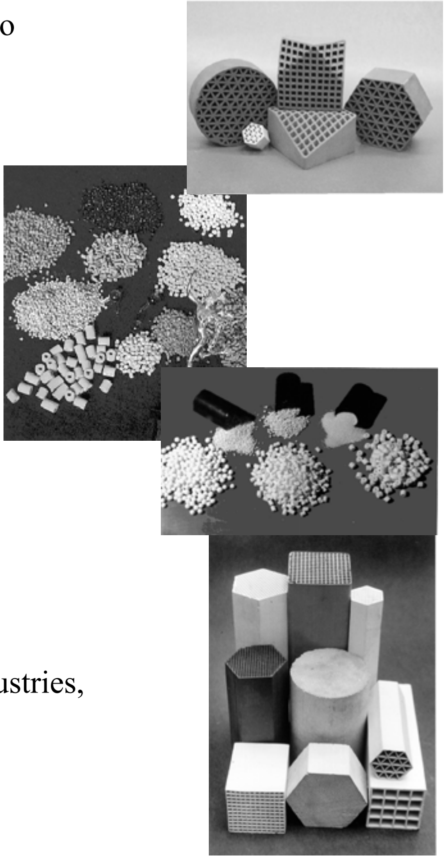
1982 REVERS-Process, USSR

Monsanto Enviro-Chem. Systems, USA, 1992

1978 Vanadium catalysts for sulfuric acid production, USSR

1958

- SOZh technology (the Claus process in aqueous solutions to remove sulfur compounds)
- Catalytic combustion using honeycomb and mat catalysts
- Synthesis of vitamins C, K and E
- Synthesis of aromatic amines and other fine organics
- HPA-based technologies
- «Chemical Heat Accumulators».



New industrial catalysts by BIC

- Catalysts for inorganic synthesis
- Catalysts for organic and fine synthesis
- Catalysts for olefin polymerization
- Catalysts for oil processing
- High silica zeolites
- Catalysts for treatment of gaseous and liquid wastes of industries, energetics, transport, etc.
- Catalysts for treatment of technological gases.

New catalyst supports by BIC

- A systematic set of alumina supports prepared through a single technology
- Catalyst supports of very high mechanical strength for fluidized and moving catalyst beds
- Mechanically strong carbon supports with adjustable porous structure
- Ceramic and carbon monoliths
- Mechanically strong supports for immobilization of enzymes
- Aerogels.

INSTRUMENT FACILITIES

The Institute engages the leading position in the world in the improvement and design of new physicochemical methods for catalyst study. Boreskov Institute of Catalysis has specialized groups united into Department of Physicochemical Methods for Catalyst Investigation oriented at analytical and scientific studies. At the Department there are many specialists of high qualification specializing in the investigation of catalysts and nanomaterials.

Modern and, in some cases, unique physicochemical methods provide a basis for fundamental studies at the atomic-molecular level.

The types of analytical and research studies performed at the Institute and methods used for them are listed below.

Analytical (composition of catalysts and catalytic reaction products)

Bulk composition

Atomic emission spectrometry
Atomic absorption spectroscopy
X-Ray fluorescence analysis of macro- and microprobes

Phase analysis

X-Ray diffraction, including *in situ* diffraction
Differential dissolution
Thermally programmed reduction, oxidation, desorption
X-Ray diffusion scattering
EXAFS spectroscopy (for amorphous materials)

Morphology

Transmission electron microscopy
High resolution transmission electron microscopy (HRTEM)
Scanning electron microscopy
Scanning tunneling microscopy
X-Ray small-angle scattering

Surface

X-Ray photoelectron spectroscopy (XPS)
Secondary ion mass-spectrometry (SIMS)
Determination of the surface acidity using IR spectroscopy of probe molecules

Molecular composition of individual compounds and their mixtures

Gas, gas-liquid and liquid chromatography on packed, capillary and polycapillary columns
Superrapid chromatography
Mass-spectrometry

Adsorptive (specific surface area, pore structure, adsorption heat)

Porosimetry
Calorimetry

Kinetic

Gradientless and integral differential reactors
Fast relaxation technique
Stop flow technique
Radiochemical and isotopic methods
Mass-spectrometric detection of free radicals.

Spectral methods

NMR spectroscopy on different nuclei, including high-temperature and *in situ*
ESR spectroscopy, including *in situ*
FMR spectroscopy, including *in situ*
VUV electron spectroscopy
UV-VIS electron spectroscopy
Vibrational spectroscopies (IR, including *in situ,* and RAMAN)
HREELS
LEED
X-Ray and NMR tomography

INTERNATIONAL COOPERATION

The scientific cooperation of the Boreskov Institute of Catalysis with the catalytic communities from various countries is effected in accordance with various forms of cooperation: conducting joint seminars on catalysis, exchanging research fellows, visiting scientific centers, and participating in congresses and symposia on theoretical and applied catalysis.

According to research programs, projects and grants, the fundamentals of catalysis are studied jointly with researchers from various universities, institutions, research laboratories and companies. BIC collaborates fruitfully on a commercial basis with the leading companies from more than 20 countries, sells licenses, know-how and performs research projects according to client requests.

Visits of the specialists from the Boreskov Institute of Catalysis to foreign institutions

Austria	30	Japan	3	South Korea	1
Belgium	1	Kazakh Republic	2	Spain	6
Canada	2	Netherlands	23	Sweden	1
China	4	Poland	5	Switzerland	2
France	8	Portugal	4	Turkey	1
Germany	49	Saudi Arabia	2	Ukraine	3
Greece	1	Slovakia	2	United Kingdom	6
India	1	Sough African Republic	1	USA	14
Italy	13				

Visits of foreign specialists to the Boreskov Institute of Catalysis

Belgium	1	Italy	3	Saudi Arabia	2
China	4	India	2	United Kingdom	5
France	8	Japan	12	USA	25
Germany	1	Netherlands	13		

SCIENTIFIC COOPERATION
WITHIN THE FRAMEWORK OF CONTRACTS AND AGREEMENTS
WITH NATIONAL SCIENTIFIC CENTERS OF FOREIGN COUNTRIES

ITALY

The cooperation in the frame of the agreement between Russian Academy of Sciences (RAS) and National Council on the Scientific Research of Italy: **Institute of Energy Conversion and Storage**, **TAE-CNR**, Messina – **BIC**, Novosibirsk, "*Catalysis for Solving the Energy Problem*".

FRANCE

According to the agreement between RAS and CNRS **BIC** collaborates with:

— **Institute de Recherches sur la Catalyse**, Villeurbanne on the BIC-IRC Twinning Programme:

- *Syngas and Hydrogen Production for Internal Combustion Engines and for Fuel Cells in Electrical Vehicles*
- *Heterogeneous Catalytic Oxidation of Organic Impurities in Waste Water*
- *Diffusion of Protons and Water in Solids and Membranes*
- *Clean Catalytic Oxidation Reactions in Fine Chemistry.*

— **Université Pierre et Marie Curie**, Paris on the project *"NMR Investigations of Supported Vanadium Catalysts"*.

INDIA

In the frame of Indo-Russian Integrated Long Term Programme of cooperation in science and technology (ILTP) BIC collaborates with

— **Central Salt&Marine Chemicals Research Institute**, Bhavnagar on the project *"Olefin Hydroformylation"*.

— **National Chemical Laboratory**, Pune on the project *"Design of Bifunctional Supported Non-Iron Catalysts for Low-Temperature Ammonia Synthesis"*.

— **Indian Institute of Chemical Technology**, Hyderabad, on the project *"Study and Development of Heterogeneous Photocatalytic Removal of Hazardous Compounds from Air and Water*".

POLAND

In the frame of RAS-PAS agreement **BIC** cooperates with the **Institute of Chemical Technology**, Glivitse on the project *"Synthesis and Utilization of Hyperporous Solids"*.

GERMANY

The cooperation in the frame of the agreement between Russian Academy of Sciences (RAS) and German Scientific Research Society (GSRS):

- **Munich Technical University**, Munich on the Project *"Study of Macrokinetics in Direct Methanol Fuel Cells with Given Layer Structure"*.
- **Fritz-Haber-Institut der MPG**, Berlin on the projects *"Study of the Catalysts for Partial Oxidation"* and *"Development of in situ Methods for Study of Solid Surfaces"*.

COOPERATION IN THE FRAME OF PROJECTS FINANCED BY INTERNATIONAL FOUNDATIONS

INTAS SUPPORTED PROJECTS

I. Novel Nanocomposites of Nanocarbons: Synthesis, Characterization, Application

Project Coordinator:

Prof. Yu. Svirko, University of Joensuu, Finland

Participants:

Dr. J-M. Bonard, Ecole Polytechnique Federale de Lausanne, Switzerland
Dr. V. Kuznetsov, Boreskov Institute of Catalysis, Novosibirsk, Russia
Dr. N. Yudanov, Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia
Dr. T. Kononenko, General Physics Institute, NSC, Moscow, Russia
Dr. A. Obraztsov, Moscow Lomonosov State University, Moscow, Russia
Dr. G. Mikheev, Institute of Applied Mechanics, Izhevsk, Russia.

II. Ethanol Combustion in a Solid Oxide Fuel Cell for Electrical Power Generation Aided Study

Project Coordinator:

Prof. P. Tsiakaras, University of Thessaly, Greece

Participants:

Prof. V. Sobyanin, Boreskov Institute of Catalysis, Novosibirsk, Russia
Dr. S. Kirillov, Institute of Technological and Information Innovations, Kiev, Ukraine
Dr. A. Demin, Institute of High Temperature Electrochemistry, Ekaterinburg, Russia
Dr. V. Antonucci, Institute of Transformation and Accumulation of Energy,
CNR, Messina, Italy.

III. Experimental and Theoretical Studies of Temporal and Spatial Self-Organization Processes in Oxidative Reactions over Platinum Group Metals. An Approach to Bridge the Gap between Single Crystals and Nano-Size Supported Catalyst Particles

Project Coordinator:

Prof. B. Nieuwenhuys, Leiden University, The Netherlands

Participants:

Prof. N. Jager, University of Bremen, Bremen, Germany
Prof. R. Imbihl, University of Hannover, Hannover, Germany
Prof. V. Gorodetskii, Boreskov Institute of Catalysis, Novosibirsk, Russia
Prof. M. Vasiliev, Physical Institute, Kiev, Ukraine
Dr. M. Slin'ko, Institute of Physical Chemistry, Moscow, Russia.

IV. Development and Study of New Catalytic Systems Based upon Microdomain Textured Perovskites for Efficient Lean DeNOx Process, CO Removal and C_2H_6 Conversion

Project Coordinator:

Prof. R. Schloegl, Fritz-Haber-Institut der MPG, Berlin, Germany

Participants:

Prof. V. Parmon, Boreskov Institute of Catalysis, Novosibirsk, Russia
Prof. N. Lyakhov, Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia
Prof. Z. Mansurov, Al'-Farabi Kazakh State University, Almaty, Kazakhstan
Prof. V. Corbean, Institute of Catalysis and Petrochemistry, Madrid, Spain.

V. The Nature of Sulfated Zirconia Strong Acidity

Project Coordinator:

Prof. J. Vedrine, University of Liverpool, Liverpool, United Kingdom

Participants:

Prof. G. van Tendeloo, University of Antwerpen RUCA, Antwerpen, Belgium
Prof. D. Kochubey, Boreskov Institute of Catalysis, Novosibirsk, Russia
Prof. A. Kokorin, Institute of Chemical Physics, Moscow, Russia
Prof. A. Kulak, Institute of General and Inorganic Chemistry, Minsk, Belarus.

VI. Catalytic Oxidation of Organic Pollutants in Waste Waters

Project Coordinator:

Dr. P. Gallezot, Institut de Recherches sur la Catalyse, Villeurbanne, France

Participants:

Prof. M. Sheintuch, Technion-Israel Institute of Technology, Haifa, Israel
Prof. V. Parmon, Boreskov Institute of Catalysis, Novosibirsk, Russia
Prof. B. Laskin, Research Scientific Center for Applied Chemistry, St. Petersburg, Russia.

VII. Advanced Highly Ordered Thermostable Nanoscale Silicates, Their Derivatives and Composite Materials

Project Coordinator:

Dr. A. Gedeon, Université Pierre et Marie Curie, Paris, France

Participants:

Dr. R. Dinnerbier, Max-Plank Institute for Solid State Research, Stuttgart, Germany
Prof. V. Fenelonov, Boreskov Institute of Catalysis, Novosibirsk, Russia
Dr. S. Kirik, Institute of Chemistry and Chemical Engineering, Krasnoyarsk, Russia.

VIII. Nanocrystalline Dense Oxide Materials as High Mixed Conductivity Membranes for Efficient Methane Conversion into Syngas by the Oxygen of Air; Fundamentals of Synthesis by Advanced Methods and Factors Determining Their Performance

Project Coordinator:

Dr. S. Neophytides, Institute of Chemical Engineering & High Temperature Processes-FORTH, Patras, Greece

Participants:

Dr. V. Zyryanov, Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia
Prof. V. Sadykov, Boreskov Institute of Catalysis, Novosibirsk, Russia
Dr. L. Ivashkevich, Research Institute for Physical and Chemical Problems, Belarus State University, Minsk, Belarus
Prof. J. Criado, Sevilla Institute of Material Sciences, Sevilla, Spain.

COPERNICUS

I. Natural Gas Fuelled Solid Oxide Fuel Cells (SOFCS) for Cogeneration of Electricity and Chemicals

Project Coordinator:

Prof. A. Payatakes, Institute of Chemical Engineering and High Temperature Chemical Processes, Rion-Achaia, Greece

Participants:

Prof. M. Ormerod, Keele University, Staffordshire, United Kingdom
Dr. A. Demin, Institute of High Temperature Electrochemistry, Ekaterinburg, Russia
Prof. Ch. Comninellis, Swiss Federal Institute of Technology, Lausanne, Switzerland
Prof. V. Sobyanin, Boreskov Institute of Catalysis, Novosibirsk, Russia
Prof. V. Kozhukharof, University of Chemical Technology and Metallurgy, Sofia, Bulgaria
Dr. N. Zakarina, Institute of Organic Catalysis and Electrochemistry, Almaty, Kazakhstan.

II. Feasibility Study of Novel Technology for Natural Gas Liquefaction Based on Plasma Catalysis and the Fischer-Tropsch Synthesis

Project Coordinator:

Prof. M. Heintze, Institut für Niedertemperatur-Plasmaphysik eV, Greiswald, Germany

Participants:

Prof. J.-M. Cormier, University of Orleans, France
Dr. B. Potapkin, Russian Research Centre “Kurchatov Institute”, Moscow, Russia
Prof. V. Kirillov, Boreskov Institute of Catalysis, Novosibirsk, Russia.

III. Recovery of Methane from Vent Gases of Coal Mines and Its Efficient Utilization as a High Temperature Heat Source

Project Coordinator:

Prof. G. Eigenberger, Institute of Chemical Process Engineering, Stuttgart University, Germany

Participants:

Prof. A. Noskov, Boreskov Institute of Catalysis, Novosibirsk, Russia
Prof. V. Babkin, Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia
Prof. K. Gosiewski, Pedagogical University of Czestochowa, Czestochowa, Poland
Prof. K. Warmuzinski, Institute of Chemical Engineering of the PAS, Gliwice, Poland
Prof. P. Forzatti, Research Group at Department of Industrial Chemistry and Chemical Engineering “Natta” at Politecnico di Milano, Milano, Italy.

IV. Development of the Environmentally Benign Technology for Deep Recovery of Elemental Sulfur from Technological Off-Gasses of Metallurgical Coke Plants and Chemical Refineries of Crude Oil

Project Coordinator:

Prof. K. Luyben, Delft University of Technology, The Netherlands.

Participants:

Prof. J. Garcia Fierro, Institute of Catalysis and Petrochemistry, Madrid, Spain
Prof. Z. Ismagilov, Boreskov Institute of Catalysis, Novosibirsk, Russia
Dr. Yu. Plyuto, Institute of Surface Chemistry National Academy of Sciences of Ukraine, Kiev, Ukraine.

NATO PROGRAMME: SCIENCE FOR PEACE

I. Catalytic and Electrochemical Processes for SO_2 and NO_x Emission Abatement

NATO Country Project Director:

Dr. S. Boghosian, Institute of Chemical Engineering and High Temperature Chemical Processes, Patras, Greece

Partner Country Project Director:

Prof. B. Bal'zhinimaev, Boreskov Institute of Catalysis, Novosibirsk, Russia.

Project Co-Directors:
Prof. R. Fehrmann, Technical University of Denmark, Denmark
Dr. V. Parvulescu, University of Bucharest, Bucharest, Romania
Dr. J. Winnick, Georgia Tech, Atlanta, USA
Mr. Yu. Zhukov, Byisk Oleum Plant, Byisk, Russia.

II. Development of Shape Steam Reforming Catalysts

NATO Country Project Director:

Prof. J.A. Mouljin, Delft Technological University, Delft, The Netherlands

Partner Country Project Director:

Prof. V. Parmon, Boreskov Institute of Catalysis, Novosibirsk, Russia

Project Co-Director:

Mr. S. Perezhogin, Ulba Metallurgical Plant, Ust-Kamenogorsk, Kazakhstan.

III. Novel Photocatalysts and Processes for Degradation of Chemical Warfare Agents

NATO Country Project Director:
Prof. P. Smirniotis, University of Cincinnati, Cincinnati, USA

Partner Country Project Director:
Dr. A. Vorontsov, Boreskov Institute of Catalysis, Novosibirsk, Russia

Project Co-Director:

Prof. R. Tsekov, University of Sofia, Sofia, Bulgaria.

IV. Synthesis of Ordered Mesoporous Aluminas and Their Application as Catalyst Supports

NATO Country Project Director:
Dr. T. Blasco, Instituto de Tecnologia Quimica, Valencia, Spain

Partner Country Project Director:
Prof. H. Caldararu, Institute of Physical Chemistry "I.G. Murgulescu", Bucharest, Romania

Project Co-Directors:

Dr. G. Pop, Zecasin S.A., Bucharest, Romania
Prof. A. Startsev, Boreskov Institute of Catalysis, Novosibirsk, Russia
Dr. J. Cejka, J. Heyrovský Institute of Physical Chemistry, Prague, Czech Republic
Ing. K. Svoboda, Chemopetrol, Litwinov, Czech Republic
Dr. M. Derewinski, Institute of Catalysis and Surface Chemistry, Krakow, Poland
Prof. A. Khan, University of Lund, Lund, Sweden.

V. Mixed Conducting Membranes for Partial Oxidation of Natural Gas to Synthesis Gas

NATO Country Project Director:

Prof. J. Frade, University of Aveiro, Aveiro, Portugal

Partner Country Project Director:

Dr. V. Kharton, Institute of Physicochemical Problems, Belarus State University, Minsk, Belarus

Project Co-Directors:

Dr. J. Irvine, School of Chemistry, University of St. Andreas, Scotland, UK
Dr. T. Norby, Centre for Material Science, University of Oslo, Oslo, Norway
Dr. J. Jurado, Institute of Ceramics and Glass, Madrid, Spain
Prof. V. Sobyanin, Boreskov Institute of Catalysis, Novosibirsk, Russia
Prof. V. Kozhevnikov, Institute of Solid State Chemistry, Ekaterinburg, Russia
Dr. L. Boginsky, Institute for Personal Development and Staff Retraining in New Areas of Techniques, Technologies and Economics of the Belarus Ministry of Education, Minsk, Belarus.

CRDF

I. Infrared Studies of Nature of Solvated Proton

Project Coordinators:

Prof. E. Stoyanov, Boreskov Institute of Catalysis, Novosibirsk, Russia
Prof. Ch. Reed, University of California, Riverside, USA.

II. Polyoxometalate - Fabric Catalysts for the Purification of Polluted Air in Human Environments

Project Coordinators:

Dr. O. Kholdeeva, Boreskov Institute of Catalysis, Novosibirsk, Russia
Dr. C. Hill, Emory University, USA

III. Catalysis by *in-situ* Generated Oxidants

Project Coordinators:

Prof. V. Bukhtiyarov, Boreskov Institute of Catalysis, Novosibirsk, Russia
Dr. W. Goodman, Texas A&M University, USA.

IV. Nanocrystalline Oxides as Novel Catalytic Materials and Destructive Sorbents for Hazardous Compounds: Relationship Between Synthesis, Structure and Reactivity

Project Coordinators:

Prof. A. Volodin, Boreskov Institute of Catalysis, Novosibirsk, Russia
Prof. K. Klabunde, Kansas State University, USA.

INTERNATIONAL SCIENCE AND TECHNOLOGY CENTER (ISTC)

I. Development of Ecological Pure Technology for Effective and Safely Treatment and Destruction of Organic and Inorganic Materials and Hazardous Wastes in Supercritical Water

Project Manager:

Prof. V. Anikeev, Boreskov Institute of Catalysis, Novosibirsk, Russia.

II. Development of a Compact Low Emission Wall-Mounted Catalytic Water Heater Boiler of 5-25 kW Power Based on the Two Stage Oxidation of Natural Gas

Project Manager:

Prof. V. Kirillov, Boreskov Institute of Catalysis, Novosibirsk, Russia.

III. Development of Compact and Economic Apparatus of Gas Conditioning for Proton Exchange Membrane Fuel Cells

Project Manager:

Prof. T. Yurieva, Boreskov Institute of Catalysis, Novosibirsk, Russia.

IV. Development of Galvanochemical Technology of Liquid Radioactive Waste Treatment with Following Immobilization of Radionuclides in Alumosilicate Glass Ceramics and Glasses

Project Manager:

Prof. Z. Ismagilov, Boreskov Institute of Catalysis, Novosibirsk, Russia.

V. Development of a Compact Unit for Steam Natural Gas Reforming Conjugated by Heat with Oxidation of Waste Anode Gas of Fuel Cells

Project Manager:

Prof. V. Kirillov, Boreskov Institute of Catalysis, Novosibirsk, Russia.

NWO–RFBR

I. Characterization and Catalytic Activity of Multivalent Cation Species Occluded in High Silica Zeolites

Project Coordinators:

Prof. R.A. van Santen, Eindhoven Technical University, Eindhoven, The Netherlands
Prof. G. Zhidomirov, Boreskov Institute of Catalysis, Novosibirsk, Russia

II. Experimental and Theoretical Studies of Non-Linear Phenomena in Catalytic Oxidation of NH_3 and Reduction of N_2O over Platinum Metal Surfaces

Project Coordinators:

Prof. B. Nieuwenhuys, Leiden University, Leiden Institute of Chemistry, Leiden, The Netherlands

Prof. V. Gorodetskii, Boreskov Institute of Catalysis, Novosibirsk, Russia

III. Nanosized Au Clusters as Novel Catalysts for Low-Temperature CO Oxidation and Selective Oxidation of Light Hydrocarbons

Project Coordinators:

Prof. B. Nieuwenhuys, Leiden University, Leiden Institute of Chemistry, Leiden, The Netherlands

Prof. V. Bukhtiyarov, Boreskov Institute of Catalysis, Novosibirsk, Russia

IV. Mechanism of the Active Surface Formation in Cu/ZnO Catalysts Characterized by SPM, EXAFS, Neutron Scattering, DFT Cluster and Surface Modelling

Project Coordinators:

Prof. A. Bliek, University of Amsterdam, Amsterdam, The Netherlands

Prof. T. Yurieva, Boreskov Institute of Catalysis, Novosibirsk, Russia

V. Microstructured Catalytic Reactors for Oxidation of Unsymmetrical Dimethylhydrazine

Project Coordinators:

Prof. J. Schouten, University of Amsterdam, Amsterdam, The Netherlands

Dr. S. Khairulin, Boreskov Institute of Catalysis, Novosibirsk, Russia

VI. Development of Oxygen-Permeable Membranes for the Conversion of Methane to Syngas

Project Coordinators:

Prof. H. Bouwmeester, University of Twente, The Netherlands

Prof. V. Parmon, Boreskov Institute of Catalysis, Novosibirsk, Russia

VII. Catalytic Partial Oxidation of Methane. Novel Approaches to the Catalysts Design and Process Study

Project Coordinators:

Prof. J. Mouljin, Delft Technological University, Delft, The Netherlands

Prof. Z. Ismagilov, Boreskov Institute of Catalysis, Novosibirsk, Russia

CONFERENCE AND EXHIBITION ACTIVITIES

Participation in exhibitions, discussion of commercial prospects of the displayed innovations illustrates the research and social activities of an institution and promotes an increase in its rating, and expanding of the potential market for new technologies and materials. Besides, the level and consumer properties of the scientific achievements may be evaluated in more realistic manner.

Our Institute, while owing numerous items in the field of applied catalysis, exercises the attending at exhibitions to promote its developments to the consumer market, to advertise its R&D activities and search for potential customers.

Solution of many specific problems requires joint efforts in order to promote its fastest accomplishing. International congresses, symposia, conferences, and seminars are most productive to familiarize scientists with innovations outside their own research and to disseminate the information about the results achieved to a wider audience. One of the directions of the scientific-organizational work carried out in the Institute is aimed on conducting conferences and seminars with the participation not only of Russian scientists and scientists from NIS, but foreign participants as well.

Extension Courses in the Field of Catalysis-II

January 27–February 2, Moscow Region, Russia

The Boreskov Institute of Catalysis and the Novosibirsk State University together with Ministry of Industry, Science and Technologies of the Russian Federation and Uncommercial Partnership "Chemical & Technological Scientific Center" (Moscow, Russia) have held the **Extension Courses** of the specialists in catalysis for the employees of the Russian industrial enterprises.

Among 34 participants – technical specialists of chemical, petrochemical and refinery enterprises, engaged in catalytic technologies and catalyst or support production: NK "LUKoil", JSC "Sibur", "PA Kirishinefteorgsintez" Ltd., JSC "Norilsk Nickel", JSC "Sibneft-Omsk Oil Refinery Plant" and JSC "Salavatnefteorgsintez", as well as companies – catalyst producers: Novokuibyshevsk Catalyst Plant corp., PJSC "Nizhegorodskie Sorbents", ZAO "Industrial Catalysts" (Ryazan) and others.

Conference Program included 18 lectures of chief specialists from academic institutes and scientific centers of Russia: A.V. Topchiev Institute of Petrochemical Synthesis, Moscow (**Prof. E. Slivinskii, Prof. V. Tretiakov, Dr. Orekhova**); N.D. Zelinsky Institute of Organic Chemistry, Moscow (**Prof. A. Lapidus, Prof. L. Kustov**); N.N. Semenov Institute of Chemical

Physics, Moscow (**Prof. O. Krylov**); Federal State Unitary Enterprise “Sintez”, Moscow (**Dr. O. Romashin, Prof. M. Flid**); Federal State Unitary Enterprise RSC “Applied Chemistry”, St. Petersburg (**Dr. I. Trukshin**); Federal State Unitary Enterprise “Electrostal Scientific-Production Association “Neorganika”, Moscow Region (**Dr. G. Dvoretskii**), Boreskov Institute of Catalysis, Novosibirsk (**Prof. V. Bukhtiyarov, Prof. Z. Ismagilov, Prof. A. Noskov, Prof. V. Sobyanin, Dr. O. Klenov, Dr. N. Pakhomov**) and Omsk Division of the Boreskov Institute of Catalysis, Omsk (**Prof. V. Likholobov, Prof. V. Duplyakin**).

The lectures cover the wide range of questions: catalysts and catalytic processes in petrochemistry and oil refining, catalysts and catalytic processes for environmental protection, modern state-of-art in chlorine industry, processes of hydrocarbon chlorination, physical methods of catalyst investigation.

Seminar “Up-to-Date State and Prospects of Industrial Implementation of Research Activities Results”

February 25-26, Novosibirsk, Russia

The Seminar was organized for the officers of academic and applied-research institutes, small-scale enterprises which activity is connected with the information security in the field of scientific researches that appears by the creation and economic utilization of research activities results.

The Seminar organizers:

- Boreskov Institute of Catalysis, Novosibirsk
- Ministry of Industry, Science and Technologies of the Russian Federation
- The Government of the Novosibirsk Region
- Informational Analytical Center of Corporative Development of Innovation Activity (Center CDIA), Moscow
- “KATAKON”, Novosibirsk

Manegers and collaborators of academic and applied-research institutes, small-scale enterprises from Vladivistok, Ulan-Ude, Krasnoyarsk, Volgograd, Omsk, Irkutsk, Tomsk, Chernogolovka, Moscow, Novosibirsk were among the 60 participants.

The lectures given by leading specialists – **I. Bortnik** (The Fund of Assistance to the Development of the Small Forms of Enterprises in the Scientific-and-Technical Sphere, Moscow), **Yu. Fomichev** (Department of Intellectual Property of Ministry of Industry and Science of RF, Moscow), **V. Zinov** (Commercialization Center ANE, Moscow), **G. Sapozhnikov** (The Government of the Novosibirsk Region, Novosibirsk), **A. Bocharov** (Department of Innovations and Commercialization of Technology of Ministry of Industry and Science of RF, Moscow), **A. Safronov** (Rospatent, Moscow), **A. Gohshtand** (JSC

“Expertise and Estimation”, Moscow), **L.N. Leksina** (Informational Analytical Center of Corporative Development of Innovation Activity (Center CDIA), Moscow), **Prof. V. Buznik** (Boreskov Institute of Catalysis, Novosibirsk), **M. Kateshova** (Innovation Center “Koltsovo”, Novosibirsk), **T. Ostertag** (State Public Scientific and Technical Library, Novosibirsk), **L. Dmitrieva** (State Public Scientific and Technical Library, Novosibirsk) concerned the state policy in the field of intellectual property legal protection, management and commercialization. Special emphasis was given to strategies for the acquisition and commercialization of new technologies, patent strategies and strategies for secrecy and trademark, technology intelligence and corporate management of intellectual property.

The innovation business and application of science achievements into the market of modern technologies in Novosibirsk region was characterized. The presentation of Russian Technology Transfer Network took place.

The Russian-American Seminar
“Advances in the Understanding and Application of Catalysts”, “AUAC-2003”
May 27-30, Moscow, Russia

The Russian-American Seminar **“Advances in the Understanding and Application of Catalysts”** was held in Moscow on May 27-30. It was organized by:

- Boreskov Institute of Catalysis, Novosibirsk
- University of California, Berkeley, USA

- Scientific Council on Catalysis of the Russian Academy of Sciences, Moscow
- N.N. Semenov Institute of Chemical Physics, Moscow

69 scientists from academic institutes and universities of Russia, Kazakhstan and 8 from Universities and companies of USA took part in the Seminar.

The Seminar program consisted of 7 plenary invited lectures, 30 oral presentations and 45 posters. Presentations were generally concentrated on the most recent advances in the following areas:

- Molecular Approaches to Design of New Homogeneous and Heterogeneous Catalysts and Processes
- Synthesis, Characterization and Evaluation of Single-Site Catalysts
- Catalytic Membranes
- Applications of Theoretical Methods for the Simulation of Catalyst Performance
- Novel Techniques for Catalyst Characterization at the Atomic Scale
- High Throughput Catalyst Screening

Plenary Lectures were given by:

S. Choi, B.J. Wood, J. Ryder, **A.T. Bell** (University of California, Berkeley, USA) – *«EXAFS Characterization of the Local Structure of Fe in Fe-ZSM-5"*. XAFS studying of the local structure of Fe in Fe-ZSM-5 prepared by solid-state exchange strongly suggests that the iron in Fe-ZSM-5 is present as isolated cations associated with framework aluminum.

V.I. Bukhtiyarov (Boreskov Institute of Catalysis, Novosibirsk, Russia) – *"Surface Science Techniques and in-situ Study of Mechanisms of Heterogeneous Catalytic Reactions"*. The capabilities of VG ESCALAB HP spectrometer to study the adsorption and mechanism of heterogeneous catalytic reactions were demonstrated in this presentation. It was shown that combination of XPS with other *in-situ* surface science techniques allows getting more convincing data about the system studied. The examples of the model studies described in the presentation unambiguously show that *in-situ* characterization of an operating catalyst is of great importance since allows elucidation of the real reaction mechanisms.

I.I. Ivanova (Lomonosov Moscow State University, Moscow, Russia) – *"In situ MAS NMR Spectroscopy in Heterogeneous Catalysis: Advances and Perspectives"*. Among *in situ* spectroscopic techniques, NMR spectroscopy is considered to be one of the most informative. The aim of the contribution was to review the advances in the *in situ* MAS NMR techniques for the unravel of the mechanisms of heterogeneous catalytic reactions.

C. Lo, **B.L. Trout** (MIT, Cambridge, USA) - *"Reactivity of Acidic Zeolites Via Quantum Chemical and Car-Parinello Molecular Dynamics Methods"*. The authors have performed a detailed investigation, via density functional theory (DFT) and constrained optimization, of the reactivity of acid sites in the zeolite chabazite and studied coupling reactions of methanol in zeolites and zeotypes. In summary, they have elucidated a new mechanism for direct ethanol formation from methanol that does not require the formation of surface methoxy groups or a dimethyl ether intermediate.

V.B. Kazansky (N.D. Zelinsky Institute of Organic Chemistry, Moscow, Russia) – *"Spectral Study of Unusual Localization and Unusual Superacidic Properties of Bivalent Cations in the Zeolites with High Si/Al Ratio in the Framework"*. Usually the catalytic properties of high silica zeolites are accounted for the shape selectivity effects connected with the porous structure of these materials. The results obtained for the first time indicate importance in addition to the shape selectivity of the specific structure of the distantly separated acid–base active sites.

V.V. Guliants, J. Al-Saeedi, V. Vasudevan (Department of Chemical and Materials Engineering, University of Cincinnati, Cincinnati, USA) – *"Mixed Mo-V-Te Oxide Catalysts for Environmentally Benign Propane Oxidation to Acrylic Acid"*. The crystal morphology, microstructure, crystal structures, bulk and surface compositions, as well as the catalytic performance of the model mixed Mo-V-Te-O catalysts in selective propane oxidation to acrylic acid was discussed.

G.I. Panov (Boreskov Institute of Catalysis, Novosibirsk, Russia) – *"Nitrous Oxide: New Oxidation Reactions in Organic Chemistry"*. This report was devoted to nitrous oxide as an alternative oxidant and presented a review on its application in both the gas-phase and liquid-phase oxidation reactions. The first successful examples of alternative liquid-phase approach as well as economic aspects of using N_2O oxidant were discussed.

2^{nd} All-Russian Seminar “Fuel Cells and Fuel Cell Power Plants”

(with international participants)

June 29–July 2, Novosibirsk, Russia

2^{nd} All-Russian Seminar *“Fuel Cells and Fuel Cell Power Plants”* was held at the House of Scientists, Novosibirsk, Russia. The Seminar was organized by the Boreskov Institute of Catalysis with assistance provided by the Ministry of Industry, Science and Technology of the Russian Federation, Ministry of Nuclear Industry of the Russian Federation, the International Scientific-Technical Center (ISTC), Scientific Council on Catalysis of Russian Academy of Sciences.

The Seminar was attended by more than 110 experts representing 30 organizations from 11 cities of Russia (including 23 participants from Moscow, 21 from Novosibirsk, 14 from Ekaterinburg, 9 from Sarov), as well as guests from the Ukraine, Kazakhstan, Japan, and the USA.

The Seminar was focused on the extremely important research and applied problem – development of highly efficient fuel cells, providing direct conversion of chemical reactions energy into electricity. It is universally recognized that in the nearest future fuel cells will become the base for new generation of power production technologies, much more efficient and environmentally safe than conventional energy industry. Fuel cells may find their application in power supply for extremely wide range of objects from mobile phones and cars to houses, industrial facilities and cities.

The Seminar was concentrated on improvement of existing and development of new technologies both in respect to fuel cells and fuel processors for conversion of hydrocarbon fuels into hydrogen.

Totally more than 80 oral lectures and poster contributions were presented at the Seminar.

The keynote lectures were given by:

- V. Rusanov, **V. Fateev** (RRC Kurchatov Institute, Moscow) – *"The Questions of Efficiency and Ecology of Fuel Cells with Proton-Exchange Membrane"*. It was stated in the lecture that such fuel cells developed in Russia give the way to successful production of pilot devices for stationary and mobile applications.
- **A. Demin** (Institute of High-Temperature Electrochemistry, Ekaterinburg) – *"SOFC: Potentialities and Actual Problems"*. The achievements in the area of solid-oxide fuel cells (SOFC) were reported. It was shown that SOFCs might become the most promising type of fuel cells for power production application. For further development of SOFC-based devices it is necessary to solve technical and design problems, mostly related to reliability of energy unit construction elements.
- A. Gulevich, V. Ruzhnikov, **N. Khramushin** (Institute of Physical Energetics, Obninsk) – *"Development of Planar Solid-Oxide Fuel Cells"*. The lecturer presented the development and experimental testing of different types of SOFCs and SOFC-based devices. It was reported that SOFC with carrying anode seems to become the most promising technology in this area.
- **N. Batalov** (Institute of High-Temperature Electrochemistry, Ekaterinburg) - *"R&D and Technologic Works, Aimed at the Improvement of Power Production Capacities and Operation Resource of Carbonate Fuel Cell"*. The results relates to detailed investigation of fuel electrode chemistry and inter-phase phenomena, search for optimal composition of oxygen electrode, experimental testing of matrix electrolyte, investigation of corrosion stability of construction materials in carbonate melts. The pilot tests of developed CFC unit show stable operation during 2100 hours with appropriate power characteristics.
- V. Sobyanin, **V. Parmon** (Boreskov Institute of Catalysis, Novosibirsk) – *"Catalysis and Fuel Cells"*. The last achievements of the Institute in the area of development of catalytic processes for fuel processors were reported. It was shown that catalysis plays the key role in conversion of various hydrocarbon fuels into hydrogen. The presentation included the description of advanced technologies developed for all stages of fuel processor: natural gas and liquid fuel convertors, CO shift and CO removal reactors, etc.
- **A. Sorokin,** G. Mirzoev (JSC "Avtovaz", Toliatti) – *"Comparable Analysis of Car Engines and Energy Installations Based on Fuel Cells"*. The questions of fuel cells application in car engines were discussed. It was stated that fuel cells may significantly increase the energy efficiency of the engine and decrease emission of toxic compounds, especially, in the regimes with low engine loading (e.g. 20% of maximum, which corresponds to typical value for the city cycle) and, therefore, their application seems to be extremely promising.

The Seminar also included discussions at "Round Table" dedicated to applied, technical and economical problems of development and application of fuel cell based energy units in Russia.

In order to speed up the development of nationally produced fuel cell power plants, participants of the Seminar proposed the Resolution. The Boreskov Institute of Catalysis should forward the Resolution of the Seminar to the Council of the Federation and the State Duma of the RF Federal Assembly, MinAtom of Russia, the RF Ministry of Industry, Science and Technologies of Russia, the Russian Academy of Sciences, etc.

“CHEMREACTOR-16”

The Institute of Catalysis of the Siberian Branch of the Academy of Science organized the first Russian conference on this subject in Novosibirsk (Russia) in 1960. Since then, the conferences devoted to Chemical Engineering in the field of chemical reactors took place in different cities of the former USSR every 3 years. They received International status in 1996. Outstanding scientists as Professor M.G. Slinko, Academician G.K. Boreskov, Academician G.I. Marchuk (Russia), Professor K.R. Westerterp (The Netherlands), Professor G. Froment (Belgium), Professor A. Renken (Switzerland) helped a great deal in the organization and formation of these conferences. The conference CHEMREACTOR-15 took place in Helsinki, Finland, in 2001.

In the year 2003 the fundamental aspects and practical application of the catalytic processes and chemical reactors, as well as the development of the novel modern technologies were discussed during the fruitful work of two conferences “CHEMREACTOR-16” – **XVI All-Russian Conference** (Kazan, Russia) and **XVI International Conference** (Berlin, Germany).

XVI All-Russian Conference on Chemical Reactors “CHEMREACTOR-16”

17-20 June, Kazan, Russia

The Conference was organized by:

- JSC TATNEFTEKHIMINVEST-HOLDING, Kazan, Tatarstan
- Boreskov Institute of Catalysis, Novosibirsk
- Kazan State Technological University, Kazan, Tatarstan
- Uncommercial Partnership "Chemical & Technological Scientific Center", Moscow
- Ministry of Industry, Science and Technologies of the Russian Federation
- Scientific Council on Catalysis RAS
- Mendeleev Russian Chemical Society

The Conference was held at a resort place located on the picturesque bank of the Great Russian River Volga, in a suburb of Kazan.

The emphasis of the Conference was made on following topics:

- Physico-Chemical and Mathematical Bases of the Processes in Chemical Reactors in Petrochemistry and Oil Processing, Polymerization and Rubber Synthesis
- Application of Aero- and Hydrodynamics for Increasing of the Efficiency of Chemical and Catalytic Reactors
- Chemical Reactors for Solution of Ecological and Energetic Problems, Including those in Oil Processing and Petrochemistry
- Intensification and Modernization of Petrochemical and Oil Processing on the Base of New Generation of Catalysts and Catalytic Technologies
- New Types of Chemical and Catalytic Processes (Reactors), including those at short Contact Times and upon Combination of Conversion and Separation.

Plenary Lectures were presented by:

V. Duplyakin, V. Doronin (Omsk Division of the Boreskov Institute of Catalysis, Omsk) – *"Development of Catalysts and Reactors for the Petroleum Refining Processes"*. The lecturer considered the interdependency of such factors as nature of crude, catalyst quality and process implementation on the example of three processes of petroleum refining – catalytic cracking, hydropurification of motor fuels and catalytic reforming of gazoline fractions.

V. Guzeev, E. Shvarev, E. Klyuzhin (Federal State Unitary Enterprise "V.A. Kargin Polymer Chemistry and Technology Research Institute with a Pilot-Production Plant", Dzerzhinsk) –

"Development of the Processes of Vinylchloride Polymerization". The lecture presented the principal technological schemes of vinylchloride production and characteristics of technological equipment. The prospects of development of each polymerization method were discussed.

A. Noskov (Boreskov Institute of Catalysis, Novosibirsk) – *"Technological Bases for Application of Structured Systems in Catalytic Processes"*. The lecture showed the prospects of application of structured systems in catalytic processes, presented the mathematical models for analysis of such systems and methods for definition of parameters of such models based on the modern physical methods.

A. Bazanov*, **B. Laskin** (*Boreskov Institute of Catalysis, Novosibirsk; Federal State Unitary Enterprise "RSC "Applied Chemistry", St. Petersburg) – *"Main Problems of Low Tonnage Chemical Industry"*. The lecture comprised the analysis of economic activity of enterprises of chemical complex of Russia. RSC "Applied Chemistry" develops work package to extend the relations between scientific and technical area and industry.

S. Dyakonov (Kazan State Technological University, Kazan, Russia) – "*Phase Equilibrium and Transition Kinetics in Multicomponent Systems Based on the Theory of Integral Equations for Partial Frequency Functions*". The lecture was devoted to the development of theoretical base of chemical processes. The possibility of the theory of integral equations for partial frequency functions for description of phase transition liquid–vapor, liquid-liquid, liquid-solid was considered.

M. Slinko (SSC "Karpov Scientific-Research Physico-Chemical Institute", Moscow, Russia) – *"Mathematical Modeling of Chemical Processes"*. Priority problems in development of up-to-date catalytic reactors was stated in the lecture.

XVI International Conference on Chemical Reactors "CHEMREACTOR-16"

Exhibition "Russian Resource-Saving and Environmental Protection Technologies"

December 1-5, Berlin, Germany

The organizers of the Conference:

- Boreskov Institute of Catalysis, Novosibirsk, Russia
- DECHEMA (Society for Chemical Engineering and Biotechnology), Germany
- Ministry of Industry, Science and Technologies of the Russian Federation
- Russian Scientific and Cultural Center in Berlin
- European Federation on Chemical Engineering
- Scientific Council on Catalysis RAS
- Russian Center of International Scientific and Cultural Cooperation of Ministry of Foreign Affairs RF

The Conference was held in Berlin, Germany, in the Russian Scientific and Cultural Center situated in the central part of Berlin.

The scientific program of the Conference comprised plenary lectures, key-note lectures, oral and poster presentations on the following topics:

- Physico-Chemical and Mathematical Bases of Processes Occurring on Catalysts Surface
- Processes in Chemical Reactors
- New Types of Chemical Processes and Reactors
- Chemical Reactors for Solving the Fuel and Energy Production Problems
- Waste Detoxication and Processing

150 participants were registered for the Conference and Exhibition. Not only scientists, but also representatives of industrial enterprises and companies engaged in chemical technology took part in the Conference and in the Exhibition. They represented 20 countries including Germany, Russia, France, Sweden, Switzerland, Italy, Spain, The Netherlands, Finland, Austria, Libia, Ukraine, Poland, Indonesia, Saudi Arabia, India, Iran, Norway, Nigeria, Japan.

5 plenary lectures, 3 key-note lectures, 55 oral contributions, 45 posters were presented.

The following scientists have presented *Plenary Lectures*:

V. Parmon (Boreskov Institute of Catalysis, Novosibirsk, Russia) – *"New Ways of Production and Utilization of N_2O"*. The presentation considered an extremely selective hydroxylation of benzene with N_2O over zeolite catalysts developed as AlphOx^{TM} process for large-scale production of phenol, as well as some other promising applications of N_2O as selective oxidant in organic synthesis.

J.-C. Charpentier (Department of Chemical Engineering/CNRS, France) – "*4 Main Objectives for the Future of Chemical and Process Engineering Mainly Concerned by the Science and Technologies of New Materials Production*". The future for the science and technologies of new materials was summarized by four main objectives: 1. A total multiscale control of the process to increase selectivity and productivity; 2. A design of novel equipment based on scientific principles and new operation modes and methods; 3. A formulation or product design and engineering: manufacturing end-use properties; 4. An implementation of the multiscale and multidisciplinary computational chemical engineering modelling and simulation to real-life situation.

G. Kolios, **G. Eigenberger** (Stuttgart University, Germany) – *"Autothermal Reactor Concepts for the Energy-Efficient Coupling of Endo- and Exothermic Reactions"*. The examples presented in the lecture show that a proper reactor design, ensuring good burner gas distribution and avoiding homogeneous back-ignition of the combustion reaction is crucial for a successful operation.

M. van Sint Annaland, J. Smit, U. Kuerten, S.A.R.K. Deshmukh**,** J.A.M. Kuipers (University of Twente, The Netherlands) – *"Development and Modelling of Membrane Reactors"*. Firstly, the benefits of controlled oxygen dozing via porous membranes to a packed catalyst bed were demonstrated. Then it was shown that with a membrane assisted fluidized bed mass heat transfer limitations can be effectively eliminated and almost isothermal conditions and plug-flow behavior can be achieved simultaneously. Finally, a new membrane reactor concept for the catalytic partial oxidation of methane with integrated air separation with oxygen perm-selective membranes was discussed.

I. Koptyug (International Tomography Center, Novosibirsk, Russia) – *"NMR Imaging: A Powerful Toolkit for Catalytic Research"*. One of the aims of presentation was to demonstrate that Magnetic Resonance Imaging is not a single research tool, but rather a sophisticated and versatile toolkit, which can provide unique and diverse information on the reactor structure and functional behavior and their interrelation.

Scientific-technical Exhibition *"Russian Resource-Saving and Environmental Protection Technologies"* was held as a part of the Conference. Organizer of the Exhibition was the Ministry of Industry, Science and Technologies of the Russian Federation.

Almost 70 complete technologies were presented. The forms of presentation were diversified: static and effective devices, experimental models, samples, subject plane-tables, advertising computer commercial films and video films.

The biggest number of technologies were presented by the leading institutes of the Siberian Branch of the Russian Academy of Sciences: Boreskov Institute of Catalysis, Kutateladze Institute of Thermal Physics, Institute of Aero-Optics, Nikolaev Institute of Inorganic Chemistry, Institute of Solid State Chemistry and Mechanochemistry.

The Exhibition demonstrated nonconventional power sources, heat- and energy-saving technologies, monitoring of the environment, technologies for purification of wastewater and treatment of off-gases of industrial enterprises, waste-handling methods and methods of radioactive decontamination.

Seminar "Polymericfluorine Materials: Fundamental, Applied and Industrial Aspects"

August 9-11, Ulan-Ude, Russia

The Conference was held at the picturesque coast of Baikal Lake in friendly and trusting environment.

The Seminar organizers:

- The Government of the Republic of Buryatia
- Siberian Branch of Russian Academy of Sciences
- Baikal Institute for Nature Management, Ulan-Ude
- Boreskov Institute of Catalysis, Novosibirsk, Russia

50 scientists from academic and applied-research institutes, universities from Moscow, Ulan-Ude, Irkutsk, Novosibirsk, Vladivostok, St. Petersburg, Yakutsk, Krasnoyarsk, Chernogolovka, Homel, as well as 6 representatives of chemical industrial enterprises from Kirovo-Chepetsk and Perm took part in the Seminar.

The Seminar Program included 5 key-note lectures, 14 oral presentations and 18 reports on following topics:

- Processes of Polymericfluorine Synthesis
- Polymericfluorine Compositions
- Structure and Morphological Characteristics of Polymericfluorines and Compositions

- New in Polymericfluorine Production and Application
- Application of Polymericfluorine Materials

Key lectures were presented by:

V. Konovalenko (JSC "Plastpolymer", St. Petersburg) - "*Polymericfluorines in Russia and Abroad. Development, Production, Consumption. Prospects of Development*"

A. Pugachev (JSC "Plastpolymer", St. Petersburg) - "*Some Aspects of Chemical and Physical Polytetrafluoroethylene Modification*"

Yu. Olkhov, **S. Allayarov,** S. Konovalikhin, T. Chernysheva (Institute of Chemical Physics, Chernogolovka, Moscow Region) - "*Effect of γ -Irradiation on the Molecular-Topologic Structure of Polytetrafluoroethylene*"

A. Kharitonov, N. Piven, R. Taege*, G. Ferrier** (Institute of Energetic Problems, Chernogolovka, Moscow Region; *Air Products, Hattingen, Germany; **Air Products, Grewe, UK) - "*Kinetics and Mechanism of Direct Polyethylene Fluorination*"

S. Gubin, M. Korobov, G. Yurkov, V. Buznik*, A. Tsvetnikov** (Kurnakov Institute of General and Inorganic Chemistry, Moscow; *Boreskov Institute of Catalysis, Novosibirsk; **Institute of Chemistry, Vladivistok) - "*Metal-Containing Nanoparticles, Stabilized in the Matrix of Ultradisperse Polytetrfluoroethylene*".

The round-table meeting on actual scientific problems and on urgent questions of production and exploitation of polymericfluorines had demonstrated the usefulness of discussions held. The experimental-industrial samples of polymericfluorine production for industry, transport and medicine were demonstrated.

Scientific Social Life

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On the eve of New Year the Governor of the Novosibirsk Region Victor Tolokonski has handed diplomas and prizes over the post-graduates and young scientists who won the research competition devoted to the 45th anniversary of the SB RAS. **Dr. Denis V. Kozlov** has got the Diploma for the series of works “Development of New Photocatalysts and Devices for Photocatalytic Air Purification. Organization of Production”.

2003 г.

премии администрации Новосибирской области молодым ученым за выдающиеся научные достижения

ДИПЛОМ

второй степени

НОМИНАЦИЯ ХИМИЯ И МАТЕРИАЛОВЕДЕНИЕ

Козлов Денис Владимирович

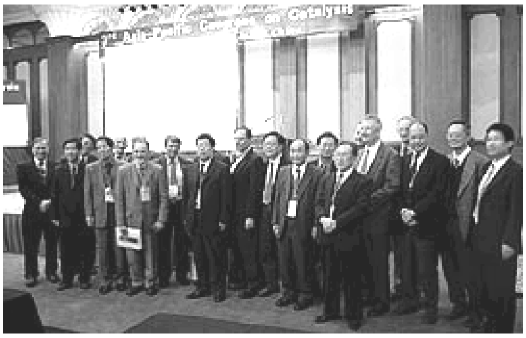
за цикл работ “Разработка новых фотокатализаторов и устройств фотокаталитической очистки воздуха. Организация производства”

Глава администрации Новосибирской области *В.А. Толоконский*

The 8th of February is designated in calendars as the Day of Russian science. It has been established in 1999 by the Russian Federation Presidential Decree in commemoration of the 275th anniversary of the Russian Academy of Sciences.

Within the framework of the **Days of Science** the meetings and excursions have been organized at the Boreskov Institute of Catalysis for the students of the Chemical Engineering College and pupils of the Grammar school. Students and pupils obtained information about modern physicochemical methods of investigation related to catalysis science, about technique of the Institute and priority directions of the Institute development.

Large-Scale Landing of the Institute of Catalysis to Innsbruck: Stately delegation of scientists (more than 40 person) of the Boreskov Institute of Catalysis participated in the regular European Congress on Catalysis "EuropaCat-6", held in Innsbruck, Austria on August 13-September 4. **Dr. O. Kholdeeva, Prof. Z. Ismagilov, Dr. A. Matveev** (joint work of the Boreskov Institute of Catalysis and Tomography Center) and **Dr. E. Melgunova** gave Oral presentations.



Large-scale event on the problems of catalysis, **“APCat-3”** (Asia - Pacific Congress on Catalysis) was held at the Chinese city of Dalian on October 12-15. **Academician V. Parmon** (the member of International Organizing Committee), **Prof. G. Panov, Prof. V. Sadykov** and **Dr. I. Yakovleva** took part in the Congress.

Professor Valerii I. Bukhtiyarov – M.A. Lavrentiev Prize 2003 winner.

November, 19, on the anniversary of outstanding Russian scientist, founder of the Siberian Branch of the USSR Academy of Sciences Academician Michail Alekseevich Lavrentiev a ceremonial meeting devoted to the M.A. Lavrentiev Prize presenting to the winners of 2003 has been held at the House of Scientists of the SB RAS. The youth M.A. Lavrentiev Prize "For Remarkable Contribution to the Development of Siberia" was awarded to **Prof. Valerii I. Bukhtiyarov**, acting director of the Boreskov Institute of Catalysis.

On **August, 4, 1997 Zamaraev International Charitable Scientific Foundation** has been organized in the memory and honor of Professor Kirill I. Zamaraev.

The main Founders of the Foundation from the Russian side are:

- Boreskov Institute of Catalysis, Novosibirsk
- Institute of Semiconductors Physics, Novosibirsk
- Russian D.I. Mendeleev Chemical Society, Moscow
- Scientific-Industrial Company «Altay», Byisk
- «Ecogeochem Ltd.», Moscow
- Association «Russian House for International Scientific and Technological Cooperation»
- Other scientific, commercial and financial institutions.

The Foundation is supported by IUPAC and some Russian sponsors.

Zamaraev Foundation is grateful to all sponsors for their contribution and invites Russian and foreign organizations (as well as wealthy persons) to become the honorary participants of the campaign.

The main aim of the Foundation is to support gifted Russian scientific youth working in the field of chemical catalysis, physical methods of its research and chemical physics.

Major part of Foundation means is spent on Zamaraev post-graduate scholarships, prizes and grants. Foundation plans to support the international cooperation of scientific youth in the field of chemical catalysis and chemical physics, i.e., their participation in international scientific conferences and seminars. **I. Mazov, A. Stadnichenko, E. Kozlova** and **I. Baturov** have got the Scholarships-2004. **Yu. Larichev, M. Grushetskaya, A. Usoltseva** and **A. Lysova** have got the post-graduate scholarships; **M. Malyshev, D. Vorobiev** and **O. Snytnikova** - incentive post-graduate scholarships.

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10 Ph.D. students and scientific employees of the Institute form the personnel of the **Council of Scientific Youth.** The main principle of the Council is submission of the interests of the youth in the Institute. It includes organization of competition of the youth projects, support of the young lecturers of higher educational establishments – employees of the Institute, organization of training for qualifying examinations for the Ph.D. degree, improvement of living conditions of the young scientists, and other directions of activity connected with the improving of a position of the young employees in the Institute.

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Memorial Rooms of Academician Georgii K. Boreskov and Academician Kirill I. Zamaraev

The **Memorial Room of Academician Georgii K. Boreskov**, the founder and first director of the Institute of Catalysis, was opened in June 1987, on the occasion of his 80th anniversary.

Georgii Konstantinovich always emphasized that the foundation of the Institute was the most important cause of his life. In 1991, the Institute of Catalysis was named after Georgii K. Boreskov.

There is a small exhibition based on the documents, awards, books, Boreskov's belongings in one of the rooms of Laboratory of Oxidation, which was headed by Georgii Konstantinovich.

A series of photos dated 1930's through 1960's tell about an extremely intense and fruitful activity of G.K. Boreskov in the fields of research and science management. He headed the Laboratory of Catalysis at the Chemicoradiological Institute (Odessa) in 1932 through 1937 (the laboratory registry dated 1931 with records by Georgii Konstantinovich concerning the preparation and characterization of vanadium catalysts was kept); the Laboratory of Catalysis at the Research Institute for Fertilizers and Insecto-Fungicides (Moscow) in 1937 through 1946, the Laboratory of Technological Catalysis at the Karpov Institute of Physical Chemistry (Moscow), and in 1958 became the Director of the Institute of Catalysis (Novosibirsk).

For his contribution to the Russian science, distinguished scientific, educational, managing and social activities, his great role in establishing the Siberian Branch of the USSR Academy of Sciences, Georgii Boreskov was awarded the Badge of Honor, three Orders of Lenin, Order of the Red Banner of Labor, Golden Medal of Hammer and Sickle, he was twice USSR State Prize winner, Ukrainian SSR State Prize winner, he was awarded the title of a Hero of Socialist Labor. Among the others, these decorations are exhibited in the Museum.

Boreskov's activity in the area of catalysis was recognized worldwide. He was a foreign member of the National Academy of Sciences of German Democratic Republic, honorary member of the New York Academy of Sciences, Doctor HONORIS CAUSA of the Wroclaw Polytechnic Institute (Poland) and of the Poitiers University (France). Government of Bulgarian Republic awarded the Order of Kirill and Mephodium to G.K. Boreskov. Visitors can see an unusual exposition displaying the full attributes of ceremonies of awarding the HONORIS CAUSA titles to Georgii Boreskov in Wroclaw in 1976 and in Poitiers in 1981, these are black mantles and caps, an ermine scarf and leather tubules for storing the Diplomas.

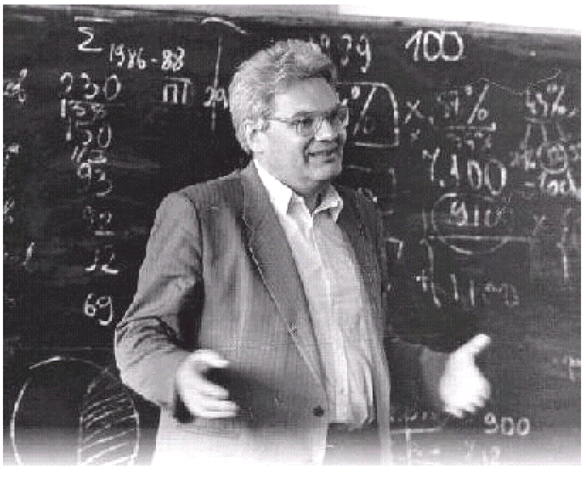
Of particular interest among the exhibit is the personal book collection of Georgii Konstantinovich including more than 1000 scientific volumes and 15 sets of Russian and foreign scientific journals. There are especially memorable copies with dedicatory inscriptions by the authors and the rarities published in the end of XIX and beginning of XX century in the collection. The books capable of telling about Boreskov's educatory activity are displayed in one of the showcases, these are course descriptions and lecture summaries, books used for preparing the lectures, and the like.

There is his writing table, case, bureau and an old push-button typewriter.

Albums, arranged by the colleagues and friends in different periods of time and presented by foreign colleagues, tell about numerous scientific events, where Boreskov presented lectures, about his keenness to winter fishing and to summer "mushroom hunting", as well as about many other interesting events.

We see the same Georgii Konstantinovich in the portraits and photos, as he was – an intellectual and charming individual.

The **Memorial Room of Academician Kirill I. Zamaraev**, the Director of the Institute of Catalysis from 1984 through 1995, was opened on the 20th of May 1999, the day of 60th anniversary of K. Zamaraev. Establishment of the Memorial Room was promoted by the International Charitable Zamaraev Foundation and directly participated by Kirill Ilyich's widow, Lyudmila Aleksandrovna Zamaraeva. This small museum exposition relates to the life and activities of Academician Kirill Ilyich Zamaraev, who was a hereditary scientist.



Diplomas, awards, photo archives and belongings of Kirill Ilyich are displayed in showcases. A unique scientific book collection gathered by him is also available here.

Kirill demonstrated his brilliant potentialities in sciences as early as his school years. He finished school as the Golden Medal winner; the medal is also stored in the Museum. He continued his education in the Mendeleev Institute of Chemical Technology in Moscow, but after the third year moved to the Moscow Physical and Technological Institute (MPhTI) in order to get a strong background in chemical physics. In the Museum, there are laboratory registries of post-graduate student Kirill Zamaraev and EPR spectra recorded by him during his post-graduate years.

The Moscow period (1956-1976) of his life and work is illustrated by the photo expositions: here is Kirill Zamaraev as a junior, then senior researcher at the Institute of Chemical Physics of the USSR Academy of Sciences; he heads a laboratory and, at the same time, he is an assistant professor in MPhTI.

Early in 1977 Kirill Ilyich was invited by Academician G.K. Boreskov; with his family and a team of young MPhTI graduates, he moved to Novosibirsk. Owing to the activity of Kirill Zamaraev and his colleagues, investigations of mechanisms of catalytic reactions at the atomic and molecular levels were considerably extended and intensified in the Institute of Catalysis.

He combined his vast research and management activity with teaching in the Novosibirsk State University.

The decade from mid-1980’s to mid-1990’s was the time of international recognition of his scientific achievements. The exhibition demonstrates his state awards, honorary medals of the USSR Academy of Sciences, as well as the certificate of full member of the USSR Academy of Sciences. He became a foreign member of Indian and Korean Academies of Sciences, awarded the Silver Medal by the Royal Chemical Society as an “Outstanding Lecturer of the Century”, and was elected a member of Academy of Europe. In 1994 K.I. Zamaraev became a President of IUPAC, International Union of Pure and Applied Chemistry, and in 1995 was honored with the German prestigious Karpinski Award for Russian Scientists. There are diplomas and medals, as well as a number of photos of that time in the Museum.

Everyone, who knew personally Kirill Ilyich, remember his exceptional ability not to loose courage at any, even very severe, circumstances. He had a really iron character, and it was not without vain that the sport he went in for was mountaineering.

A smiling, talented, brilliant and courageous man appears before visitors to the Memorial Room.

IMPORTANT RESULTS
OF THE R&D ACTIVITY

Laboratory of Quantum Chemistry
Head: Dr. Igor L. Zilberberg

- 1. Prof. V.P. Zhdanov has published a series of works extending the conceptual basis of theoretical electrochemistry. The key novel findings obtained are as follows:

(i) The effect of fluctuations of the potential near the reactants may be especially important for polymer electrolytes. In this case, due to fluctuations, the reaction rate may be enhanced by a factor of 15 compared to the mean-field value.

(ii) With realistic values of lateral adsorbate-adsorbate interactions (about 1 kcal/mol) the kinetics of electrocatalytic oxidation of CO on Pt may be accompanied by CO segregation provided that surface CO diffusion is fast.

(iii) Due to specific distribution of the electric field the rate of electrochemical reaction occurring on supported nm-sized particles may be higher (by a factor of 5) than on the flat surface.

(iv) The kinetics of CO oxidation on nm-sized supported particles may depend on the CO-diffusion-mediated communication between the (111) and (100) facets.

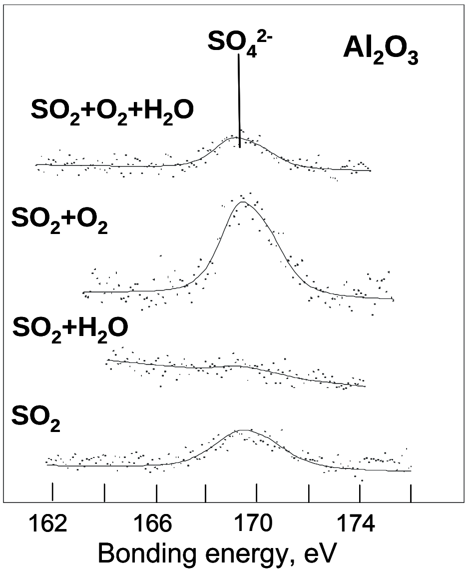
(v) In electrochemical reactions occurring on metal catalyst particles contacting simultaneously the ion-conducting electrolyte and gas phase, the deviations from the Tafel law in the dependence of the reaction rate on the electrode potential may be related to diffusion of one of the adsorbed reactants along the surface.

2. The electron structure of atomic oxygen adsorbates is studied by means of the density functional theory in the context of the ethylene epoxidation on the silver surface. The adsorption oxygen species are modeled by the Ag_2O molecule in the closed ($^1A_1$) and open-shell states ($^3B_1$ and $^1B_1$). In both open-shell states the 1s level appears to be lower than that in $^1A_1$ by about 2 eV. This is apparently a sequence of the separation of electron pair, occupying the π^*-type highest occupied molecular orbital (HOMO), decreasing the electron density at the oxygen center. Such variation of the O1s level for closed and open-shell Ag_2O states seems to explain the X-Ray photoelectron spectroscopy (XPS) data concerning two distinct atomic oxygen species on silver surface having the O1s binding energy of about 528 and 530 eV, called nucleophilic and electrophilic oxygen, respectively. The X-Ray absorption O *K*-edge spectra (XANES) calculated for two types of the Ag_2O states by means of multiple-scattered-Xα-based approach appears to be in a qualitative agreement with those experimentally recorded for nucleophilic and electrophilic oxygen.

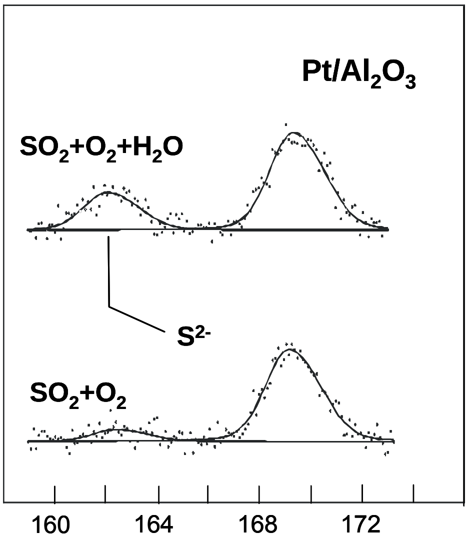
Surface Science Laboratory
Head: Prof. Valerii I. Bukhtiyarov

- In order to understand more comprehensively the mechanism of SO_2-poisoning of automobile exhaust gas neutralizing catalysts, interaction of SO_2-containing gaseous media with alumina, ceria and platinum deposited on the surface of these oxides was studied in the temperature interval of 30-400 °C and the total pressure of the gaseous reactants in the range of 2-8 Torr using XPS.

It was shown that the reaction of SO_2 with the model supported platinum catalysts results in sulfation of the oxide support and produces sulfide on the surface of platinum particles. Among two oxides studied, ceria is sulfated more efficiently, and the process is accompanied by reduction of CeO_2 into Ce(III) sulfate. At the same time, the catalyst Pt/CeO_2 is subjected to sulphidation in a lesser extent, especially at elevated temperatures. A relatively facile migration of oxygen from the lattice of CeO_2 onto the platinum surface could be the reason of the increased resistance of the catalysts against sulphidation. The efficiency of support sulfation decreases in the presence of water vapour, especially in the case of alumina support where sulfation is suppressed even in the presence of oxygen. However, water vapor has a stabilizing effect on sulfide produced on the surface of supported platinum particles.



H_2O suppresses sulfation over Al_2O_3



H_2O has a stabilizing effect on platinum sulfide

Laboratory of Investigation of the Mechanisms of Catalytic Reactions

Head: Prof. Eugenii P. Talsi

➢ *1. Relation between the structure of active intermediates and polymerization activity of catalytic system zirconocene/MAO.*

In the past two decades, catalytic metallocene/MAO systems have attracted particular attention of researchers who deal with olefin polymerization. The interest in these systems is underlain by the high activity and stability of the active centers of polymerization and unique properties of the synthesized polymers. Elucidation of the mechanism of activation of metallocenes with methylaluminoxane (MAO) needs information on the structure of the cation-like intermediates, formed upon activation of zirconocenes with MAO. It has been commonly accepted until recently that the complex and poorly understood structure of the activator (MAO) makes it impossible to obtain this kind of information.

However, BIC scientists have contributed to destroying the myth. They have demonstrated that the cationic parts of ion pairs generated during the activation of zirconocenes with MAO can be characterized in detail using ^1H and ^{13}C NMR spectroscopy. A series of papers published in 2003 report ^1H and ^{13}C NMR studies on the cation intermediates generated on activation of zirconocenes L_2ZrCl_2 with MAO in toluene at the Al/Zr ratios of 50 to 1000 (L_2 are various ligands, namely cyclopentadienyl (Cp), indenyl (Ind) and fluorenyl (Flu)). The following catalysts have been studied: $(Cp\text{-}R)_2ZrCl_2$ (R = Me, 1,2-Me_2, 1,2,3-Me_3, 1,2,4-Me_3, Me_4, Me_5, *n*Bu, *t*Bu), rac-ethanediyl$(Ind)_2ZrCl_2$, rac-$Me_2Si(Ind)_2ZrCl_2$, rac-$Me_2Si(1\text{-}Ind\text{-}2\text{-}Me)_2ZrCl_2$, rac-ethanediyl$(1\text{-}Ind\text{-}4,5,6,7\text{-}H_4)_2ZrCl_2$, $(Ind\text{-}2\text{-}Me)_2ZrCl_2$, $Me_2C(Cp)(Flu)ZrCl_2$, $Me_2C(Cp\text{-}3\text{-}Me)(Flu)ZrCl_2$, $Me_2Si(Flu)_2ZrCl_2$. Zwitter-ionic intermediates $(Cp\text{-}R)_2ZrMe^+\leftarrow Me^-\text{-}Al\equiv MAO$ (**IV**) with different anion fragments $Me\text{-}MAO^-$ have been identified in catalytic systems $(Cp\text{-}R)_2ZrCl_2/MAO$ (R=*n*Bu, *t*Bu) at low Al/Zr ratios (50–200). At high Al/Zr ratios (500–1000), intermediates $[L_2Zr(\mu\text{-}Me)_2AlMe_2]^+Me\text{-}MAO^-$(**III**) predominate in most of the systems under study. The catalytic activities of systems $(Cp\text{-}R)_2ZrCl_2/MAO$ (R = H, Me, 1,2-Me_2, 1,2,3-Me_3, 1,2,4-Me_3, Me_4, Me_5, *n*Bu, *t*Bu) and rac-$Me_2Si(Ind)_2ZrCl_2$ towards ethene polymerization correlate with concentration of intermediate **III** in the reaction system. Hence, **III** is the main precursor of active centers of polymerization in catalytic systems zirconocene/MAO.

2. The mechanism of asymmetric epoxidation of olefins with iodosobenzene catalyzed by Cr^{III}(salen)Cl

In the recent years, intensive studies have been focused on catalytic systems based on chromium complexes with chiral Shiff bases. The catalysts are used for asymmetric epoxidation of alkenes, kinetic resolution of epoxides, asymmetric Diels-Alder reactions. However, the mechanism is not as yet understood in detail. In the present study, EPR, ^1H, ^2H NMR spectroscopies are used to identify the intermediates generated during interaction of iodosobenzene with chromium(III) (S,S)-(+)-N,N′-bis(3,5-di-tert-butylsalicylidene)-1,2-cyclohexanediamine chloride (**1**) and racemic chromium(III) N,N′-bis(3,4,5,6-tetra-deuterosalicylidene)-di-tert-butylsalicylidene)-1,2-cyclohexanediamine chloride (**2**). These intermediates are the active oxocomplexes Cr^VO(salen)L (L = Cl^- or solvent molecule) and an inactive binuclear intermediate L_1(salen)$Cr^{III}OCr^V$(salen)L_2 (L_1, L_2 = Cl^- or solvent molecule) which behave as a reservoir for the active species Cr^VO(salen)L. Addition of donor molecules (DMSO, DMF, H_2O) results in an increase of Cr^VO(salen)L relative concentration over that of L_1(salen)$Cr^{III}OCr^V$(salen)L_2. The reactivity of Cr^VO(salen)L towards E-β-methylstyrene is probed.

3. Detection and characterization of alkylperoxo complexes of molybdenum

Molybdenum-catalyzed epoxidation of olefins with organic hydroperoxides remains among the most used industrial methods for production of propylene oxide and an appropriate laboratory method for epoxidation of more complex olefins. It is commonly accepted that molybdenum alkylperoxo complexes are the active species in these reactions. However, the molybdenum alkylperoxo complexes have not been yet identified or characterized spectroscopically. In 2003, the molybdenum(VI) alkylperoxo complex, which is produced on interaction between tert-butyl hydroperoxide and 1,2-cyclohexanediol complex of molybdenum(VI) and behaves as the key intermediate for catalytic epoxidation of cyclohexene, was for the first time identified and characterized using ^{13}C, ^{17}O and ^{95}Mo NMR spectroscopy.

Group of Low Temperature Catalysis by Metals
Head: Prof. Vladimir V. Gorodetskii

➢ The semi-empirical Method of Interacting Bonds was used in the present work. Various single crystal planes of Pt, Rh, Ir, Fe, and Re were examined with respect to the stability of the adsorbed NH_n species (n = 0; 1; 2; 3); to the reactivity of NH_n (n = 0; 1; 2) species towards adsorbed hydrogen atoms; and to the possibility of proceeding the combination reactions between two NH or two NH_2 particles resulting in the formation of gaseous H_2 and N_2 molecules. All the surfaces studied were found to form readily the stable NH species. This result is consistent with an earlier suggested mechanism for the oscillatory behavior that attributes the surface wave propagation to the intermediate formation of NH species. Stable NH_2 species can be formed on Re and Fe surfaces, whereas the noble metal surfaces can form weakly stable NH_2 particles at the very edge of their existence region. The combination reaction between two NH_2 species is endothermic in all cases.

The electronic peculiarity of the Pt(100)–(1×1) surface effected by various adsorbates and interaction in adsorbed layer was studied by Disappearance Potential Spectroscopy (DAPS). Two types of features were developed in DAPS spectra. The first type corresponds to an ordinary threshold excitation of platinum core electron to an available vacant state. Locations of the respective spectral satellites are close to corresponding ionization potentials of a given species in adsorbed layer. Our experimental data show altogether more than 10 satellites providing the reliability of the conjugate electron excitation process to proceed. The present results as a whole testify experimentally to the substantial unity of the substrate and adsorbate electronic structure.

The NO + CO reaction was investigated on the Pd(110) and Pt(100) surfaces by means of TPR, HREELS and molecular beam doser techniques. It was shown, that the reaction has an "explosive" character, like on the earlier studied Pt(100) and Pd(100) single crystal surfaces. Preadsorption of oxygen on Pd(110) surface has a dramatic effect on the $CO_{ads} + NO_{ads}$ reaction at low O_{ads} coverage. TPR spectra show the appearance of a new CO_2 peak at 265 K, which indicates, that at low temperatures CO favorably reacts with adsorbed oxygen. CO_2 molecules desorb perpendicularly to the surface and N_2 molecules have a desorption angle of about 30^0. By adding of $^{18}O_2$ in the system we could compare the angular distribution of N_2, NO^{18}, N_2O and the different kinds of CO_2 (CO_{ads} + $^{18}O_{ads}$; CO_{ads} + NO_{ads}). Both kinds of CO_2 molecules desorb almost perpendicularly to the surface. N_2, N_2O and NO^{18} molecules have a desorption angle of about 30° to the surface.

The decomposition and oxidation of NH_3 have been studied on the Ru(0001) surface in the temperature range from 150 K up to 800 K. The products of ammonia oxidation observed were N_2, H_2O and N_2O. Formation of NO was not found.

On Ir tips, oscillations are manifested by regular variations of the emission current as a result of moving waves that spread across a (510), (100) surfaces of the tip. The concentric waves start only at the (510) stepped nanoplanes and travel to (100) surface. Other planes, notably (110), (210) and (111) do not take part in the moving waves. The temperature range in which fast concentric waves are found is near 480 K with a NO pressure ~10^{-7} torr and NO/H_2 ratio of 10/1. Our FEM results indicated a key role of stepped surfaces in initiation of such oscillations. The principal result of this work lies in the following: the appearance of regular waves is an amazing example of self-organization of a catalytic reaction on a metal particle size of some hundreds Å.

Group of Scanning Spectroscopy
Head: Dr. Alexey N. Salanov

- Mechanisms of the reconstruction of the surface and subsurface layers of Pd(110), induced by oxygen chemisorption at pressures 10^{-6}–100 Pa and temperatures of the sample 300–1200 K were ascertained.

Group of Solid-State NMR Spectroscopy
Head: Prof. Olga B. Lapina

- The solid-state HETCOR method is adapted for spin 1/2 nuclei (^{13}C) and for quadrupolar nuclei (^{27}Al). The HETCOR technique (HETeronuclear CORrelation) is a kind of classical correlation two-dimensional spectroscopy that allows the occurrence of chemical bonds between magnetic heteronuclei to be identified. HETCOR is based on the known method of cross-polarization of nucleus magnetic moments.

Implementation of this technique seems important for the following reasons. When acquired under ordinary conditions, a NMR spectrum is a superposition of lines related to magnetic nuclei in different chemical environments. In complex systems, a considerable part of information in one-dimensional spectra is lost because of overlapping of lines with close chemical shifts. When a catalyst structure is studied, the data on the presence of bonds with certain atoms are of importance along with the information about the type of local environment of the magnetic nuclei. The surface hydroxyl groups are important to catalysis. Among the principal targets of the HETCOR technique is to understand which of surface sites is bonded with the hydroxyls. It is not always possible to identify bonds with hydrogen atoms using the one-dimensional CP-MAS technique; that is so in the case of quadrupole nuclei (^{51}V, ^{27}Al) that have relatively small relaxation times. In contrast to CP-MAS, the HETCOR technique allows a correlation spectrum to be acquired that demonstrates relations between magnetic nuclei, for example ^{13}C-^{1}H and ^{27}Al-^{1}H.

Laboratory of Texture Studies
Head: Prof. Vladimir B. Fenelonov

- The method for synthesis of thermohydrostable mesoporous silicate mesophases with a regular honeycomb structure (of the type of MCM-41, SBA-3 and SBA-15) in a wide range of pH of the medium was adopted using sodium silicate as the source of SiO_2. Stable titanium-silicate catalysts Ti-MMM-2, which are highly active and selective for oxidation of trimethylbenzene and other substrates with hydrogen peroxide, were synthesized (in cooperation with Group of Stereoselective Catalysis). Mesostructured carbon and composite carbon-mineral materials with adjustable structural and textural parameters were prepared based on the aluminosilicate mesophase SBA-15.

It was found possible to improve thermal stability and structural ordering of the mesophases using repeated hydrothermal treatment of the synthesized mesophases in ammonia solutions.

The studies of a number of microporous carbons and CFC revealed that these materials are inappropriate for storage of H_2 at room temperature and pressures up to 60–80 atm.

Group of NMR Spectroscopy for Catalytic Hydrocarbon Conversion
Head: Dr. Alexander G. Stepanov

- Kinetics of a double bond shift reaction, hydrogen exchange and the ^{13}C-label scrambling was monitored *in situ* by ^{2}H, ^{1}H and ^{13}C MAS NMR for n-but-1-ene adsorbed on zeolite ferrierite under conditions of batch reactor at 290–373 K. A double-bond-shift reaction, the fastest among the three reaction studied, can be monitored provided that 98 % of Brønsted acid sites are substituted by Na cations. The activation energy for the reaction was found to be 9.8±1.1 kcal/mol. Hydrogen exchange is observed for both methene and methyl groups of n-but-2-ene, rapidly formed from the initial n-but-1-ene. Terminal olefinic $=CH_2$ group of n-but-1-ene is involved in the exchange, providing the pathway for the exchange into the methyl group of the n-but-2-ene, mainly observed in the spectrum in accord with thermodynamic equilibrium constant between n-but-1-ene and n-but-2-ene. This offers similar apparent activation energies for the exchange into methene (6.5±1.7 kcal/mol) and methyl groups (7.1±1.3 kcal/mol) of n-but-2-ene. The ^{13}C-label scrambling in n-but-2-ene is indicative of sec-butyl cation formation from the olefin in the zeolite framework, which can be formed as a small quantity transient species not detectable by NMR but providing the label scrambling. The apparent activation energy for the ^{13}C-label scrambling was found to be 20±2 kcal/mol, that is three times higher compared to the activation energy for the label scrambling in sec-butyl cation in superacidic solution.

Dr. Vitalii S. Muzykantov

➢ A new approach to characterization of mobility and reactivity of oxygen of oxide catalysts by analysis of the isotope exchange data is developed.

Transformation of strict isotopic-kinetic equations reflecting time dependence of isotope variables leads to the ratio, which does not contain time and establishes the universal relation between isotope variables (isotopic-mechanistic equation). This relation allows to derive form experimental data the mechanism parameters (types of atoms rearrangement) even for the cases of non-isothermal experiments.

Analysis of the mode of isotope redistribution between the gas-phase dioxygen and solid oxide allows to determine the amount of exchangeable oxygen and estimate its mobility. Mechanism parameters derived from redistribution of the isotope dioxygen molecules help to elucidate atomicity of intermediate particles, the nature of occurring stages and ratio of their rates.

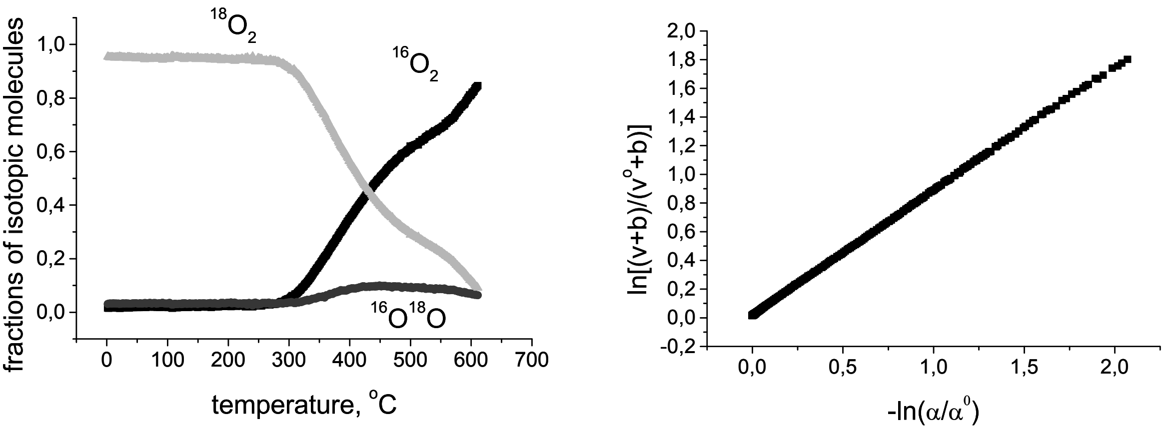
For the first time the isothermal and non-isothermal (temperature-programmed) experiments were combined. Suggested method was applied for analysis of isotope exchange data for a number of complex oxide catalysts with fluorite-like and perovskite-like structures being of great interest as solid electrolytes, mixed ionic-electronic conductors and active components of catalysts for selective oxidation of hydrocarbons by oxygen into syngas**.**

Isotopic-kinetic equation

Isotopic-mechanistic equation

$$\begin{aligned}(N/R)\,(ds/dt) &= -\,(1+\lambda)\,a_1\,s \quad (1)\\ (N/R)\,(dz/dt) &= -\,z + a_2\,s \quad (2)\end{aligned} \quad \left(\frac{(2)}{(1)}\right) \Rightarrow \quad dz/ds = (z/s)/[(1+\lambda)\,a_1] - s\,a_2/[(1+\lambda)\,a_1]$$

Application of isotopic-mechanistic equation for non-isothermal isotope exchange of dioxygen with solid oxides



Laboratory of Catalytic Methods of Solar Energy Conversion

Head: Acad. Valentin N. Parmon

- Physico-chemical transformations of aluminium hydroxide (III) under very rapid heating in a Centrifugal Flash Reactor have been investigated. So called “CTA product” has been obtained. It has a highly defective structure and possesses a high reactivity. Representative batches of a CTA product with the complete decomposition of the initial substance were prepared and used for synthesis of an active alumina of γ-, η- and α-type. The movement of gibbsite particles along the heating surface of the Reactor has been studied with the aim of the set-up optimization.

Laboratory of Energy Accumulating Materials

Head: Prof. Yurii I. Aristov

- 1. New composite sorbents based on magnesium, sodium and copper sulfates confined to mesopores of silica KSK and alumna were synthesized and investigated. Isobars of water sorption on these sorbents were measured at pressure range of 10 to 50 mbar and temperature range of 20 to 300 °C. It was shown that the sorption equilibrium and phase composition of the confined sulfates strongly depend on the salt content. At low content, the salt is stabilized in pores in XRD-amorphous phase, and the composition of its hydrated form gradually changes with the water vapour pressure and temperature (so called bivariant equilibrium). At high content, a crystalline phase of the confined salt is formed, and the sorption of water vapour is accompanied by the formation of the salt crystal hydrates with a fixed composition (monovariant equilibrium).

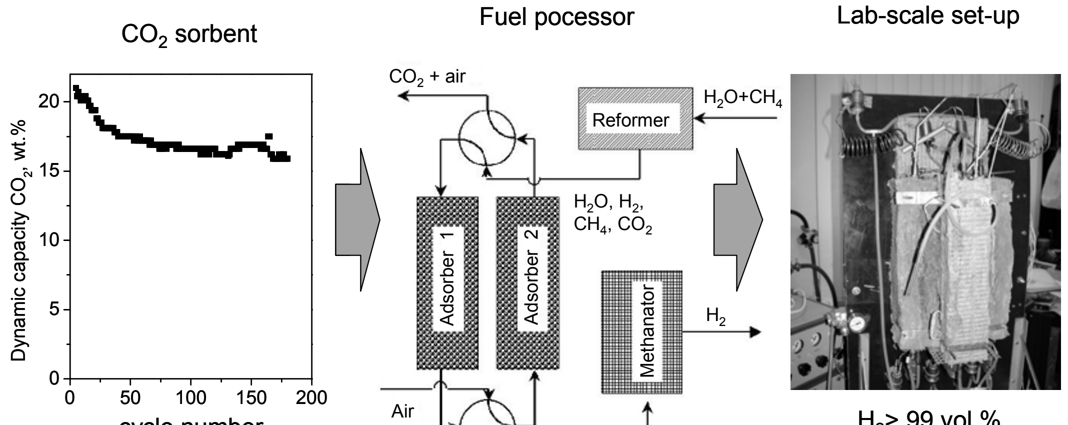
2. A mechanism for CO_2 sorption in the presence of water vapour by the $K_2CO_3/\gamma\text{-}Al_2O_3$ sorbent is studied to find out reasons responsible for a decrease in its dynamic sorption capacity during multi-cycle tests. A key role of the salt crystalline hydrates for rapid CO_2 sorption is revealed by an IR spectroscopy *in situ.* It is shown, that the decrease in the sorption capacity after a number of sorption–regeneration cycles is due to the formation of an inactive phase of potassium aluminate. After the first ten “sorption—regeneration” cycles the capacity decreases down to 35 mg/g in temperature range 20–80 °C.

3. The phase composition of calcium chloride confined to mesoporous silica was studied by differential dissolution and X-Ray diffraction techniques at various salt contents. Isobars of water sorption on these sorbents were measured at pressure range of 10 to 50 mbar and temperature range of 20 to 200 °C by TG method. It was shown that the salt forms two phases in pores, namely, crystalline bulk phase and X-Ray amorphous one. The fraction of the crystalline phase grows with increasing salt content. The sorption equilibrium was found to be sensitive to the ratio between the crystalline and X-Ray amorphous phases. It was demonstrated that at high salt content the sorption equilibrium is monovariant. At low content the composition of the confine hydrated phase changes continuously, which is typical for solutions of salts or their hydrates with a vacancy structure.

4. The main aspect of this series of work was to find out the optimum pellet size of selective water sorbents for their application in sorption heat pumps. An experimental investigation on the influence of the pellet size of SWS-1L, made by impregnating mesoporous silica with 33.7 wt. % of $CaCl_2$, on the kinetics of water vapor sorption has been done. Four samples having different pellet sizes have been prepared; namely, 0.34–0.5 / 0.71–1.0 / 1.3–1.6 and 3.0–3.2 mm. The measurements have been carried out on 3 g samples of loose pellets on an isothermal plate under three different conditions typical for the operation of sorption heat pumps. The results obtained evidence a remarkable enhancement of the kinetics of adsorption with the decrease in the pellet size.

5. It was found that alkali carbonate melt promotes CaO carbonization. This effect was used to develop a new family of CO_2 sorbents promising for temperature range 500–800 °C. A pelletized shape of the sorbent fits well common fixed bed separation processes. The sorption capacity of the novel adsorbents remains unchanged under humid environment that favors their use in sorption enhanced steam reforming of CO and hydrocarbons.

New CO_2 adsorbents were used to develop a sorption enhanced process of pure hydrogen production via catalytic steam reforming of hydrocarbons. The process comprises three main stages: hydrocarbon steam reforming, sorption enhanced CO steam reforming and methanation. Its feasibility has been tested with lab-scale set-up, producing 18 ndm^3 H_2/h starting from 33 vol. % aqueous ethanol solution as a feed. The purity of the hydrogen rich gas ($H_2 > 99$ %, $CH_4 < 1$ %, $CO_x < 100$ ppm) obtained in the tests was sufficient for feeding low-temperature fuel cells.



Group of Aerosol Catalysis
Head: Dr. Valerii N. Snytnikov

- A subsonic gas dynamic reactor with laser control of chemical reactions was made, mounted and experiments were started. Principal opportunity of realization of reaction of methane dimerization to ethylene with selectivity 100 % at millisecond contact times in the gas dynamic reactor with laser control of chemical reactions has been shown. Search for optimal regimes of reactor operation has been started experimentally as well as by mathematical modeling.

Method of instabilities studies based on estimation of scattering stochastic trajectories (PIC -method) has been proposed for many-particle systems in a self-consistent fields (gravity, electromagnetic). The method allows to establish: space and time boundaries for instability, averaged for all particle increments and increments for separate space groups, including single particle. The method makes it possible to determine average macroscopic functions in the system for the moment of instability development.

Group of Boiocatalysis
Head: Dr. Galina A. Kovalenko

- Systematic studies of adsorptive immobilization of *glucoamylase* and *invertase* enzymes on macrostructured carbon-containing ceramic supports were aimed at development of highly stable biocatalysts for the heterogeneous processes of production of starch treacle and invert sugar syrups. The carbon layer with loose and rough surface formed by catalytic filamentous carbon (CFC) was shown to possess the optimal morphology for effective adsorption and stabilization of the enzymes under study, whereas the enzymes immobilized on smooth graphite-like carbon layer were relatively low stable. In the case of invertase, the morphology of carbon layer also significantly influenced the activity of the immobilized enzyme. Invertase, adsorbed on CFC-containing ceramics retained its activity highest possible, whereas adsorption on graphite-like carbon layer resulted in complete deactivation of the enzyme.

A *rotor-inertial bioreactor RIB* was developed and designed to enhance considerably the efficiency of biocatalytic processes in which diffusion of the substrate to the enzyme immobilized on the porous supports was the limiting stage. The bioreactor was investigated in the heterogeneous process of enzymatic hydrolysis of dextrinized starch into starch treacle and glucose syrups performed by glucoamylase immobilized by CFC-coated foam-like ceramics. Under optimal conditions, RIB was shown to be 1.5–2 times as efficient as a traditional flow fixed-bed bioreactor. In the closed mode of RIB operation, the observed activity of the heterogeneous biocatalyst was 3–3.5 times higher than that in the fixed-bed bioreactor with circulation.

Group of Stereoselective Catalysis
Head: Dr. Oxana A. Kholdeeva

- The new titaniummonosubstituted polyoxometalate (Ti-POMs) of the Keggin structure, namely, μ-oxodimer $[Bu_4N]_8[(PTiW_{11}O_{39})_2O]$ (**1**) and monomeric $[Bu_4N]_4[PTi(OH)W_{11}O_{39}]$ (**2**), as well as methoxyderivative $[Bu_4N]_4[PTi(OMe)W_{11}O_{39}]$ (**3**), have been synthesized starting form the μ-hydroxodimer $[Bu_4N]_7[(PTiW_{11}O_{39})_2OH]$ (**4**). The new compounds have been characterized by using elemental analyses, IR, and ^{31}P, ^{1}H и ^{183}W NMR. Interaction of **1-4** with H_2O, H_2O_2 and 2,3,6-trimethylphenol (TMP) in MeCN has been studied and the corresponding initial rates and equilibrium constants have been estimated. ^{31}P NMR and IR studies revealed that all the Ti-POMs gave the same protonated peroxocomplex $[Bu_4N]_4[HPTi(O_2)W_{11}O_{39}]$ (**I**) upon interaction with aqueous H_2O_2. Using D_2O_2 instead of H_2O_2 a deuteroperoxocomplex $[Bu_4N]_4[PTi(OOD)W_{11}O_{39}]$

(**1-D**) has been prepared. A comparative study of **I** and **I-D** by means of IR and NMR spectroscopy revealed that the proton in solid **I** is localized at a Ti-O-W bridging oxygen rather than at the peroxo oxygen. In MeCN, the proton is delocalized between bridging Ti-O-W oxygens and the peroxo group. DFT calculations carried out by the collaborators from the Spanish group (Xavier López and Josep M. Poblet, Departament de Química Física i Inorgànica, Universitat Rovira i Virgili, Tarragona, Spain) strongly support this conclusion. The activity of the Ti-POMs in TMP oxidation with H_2O_2 in MeCN under turnover conditions was found to correlate with the peroxo complex formation rate and fall in the series **2** > **1** ~ **4** > **3**. In turn, the rates of the formation of **I** correlate with the rates of hydrolysis of **1** and **3** leading to **2**. The main products of the TMP oxidation with H_2O_2 in the presence of Ti-POMs are the same as in the case of the TMP oxidation over mesoporous Ti,Si-catalysts, namely, trimethyl-p-benzoquinone and 2,2',3,3',5,5'-hexamethyl-4,4'-biphenol. Kinetics of the TMP oxidation with H_2O_2 catalysed by **3** has been studied. The reaction is first order in H_2O_2 and the catalyst and fractional (1-0) order in TMP. The same kinetic law was found previously for the TMP oxidation with H_2O_2 over mesoporous titanium-silicate catalysts. The common features found for both Ti-POMs and Ti,Si-catalysts confirmed that transition-metal substituted POMs can be used as soluble model compound for studying catalytic action mechanisms of redox molecular sieves.

Group of Energy-Chemical Technologies

Head: Prof. Vladimir I. Anikeev

- Kinetics of nitromethane (NM), nitroethane (NE) and 1-nitropropane (NP) decomposition and oxidation in supercritical water (SCW) near the critical point have been studied. Effect of pressure on the decomposition rate of NM, NE and NP in SCW was investigated at constant temperature, activation volumes of reaction have been found. Correlation between the reactionary of the aliphatic nitrocompounds in decomposition and oxidation reactions with the number of carbon atoms was found.

The transition state theory has been applied to simulate the pressure effects. Some ideas on the nature of active complex have been suggested. The calculated values of activation volumes in the reactions of decomposition of NM, NE and NP in SCW were similar.

Mathematical modeling and optimization of technological scheme for the oxidation of organic impurities in SCW has been accomplished. Created mathematical models consider the specific properties of chemical processes realized in supercritical conditions: thermodynamic properties change (change of heat capacity, enthalpy and critical parameters of mixture with pressure, temperature and composition). Calculation results formed the basis of the pilot plant.

Group of Photocatalysis on Semiconductors

Head: Dr. Alexander V. Vorontsov

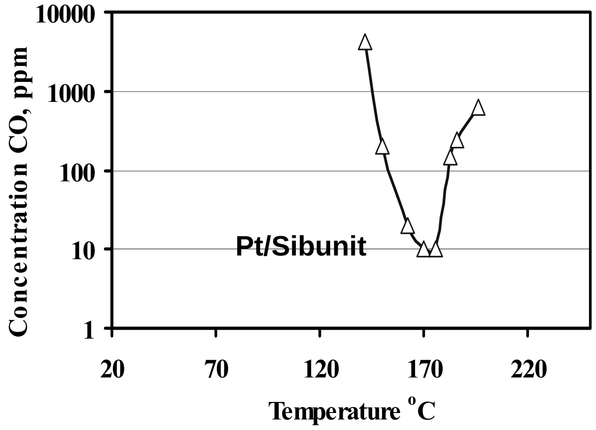
- In 2003 the laboratory of photocatalysis conducted research on photocatalytic oxidation of several organic compounds containing phosphorus and sulfur atoms, developed new photocatalysts for oxidation in liquid and gas phase, studied oxidation over heterogeneous Fenton catalysts, and commercialized air purification units for automobiles and small rooms. It has been demonstrated that oxidation of dimethylmethylphosphonate, trimethylphosphate, triethylphosphate proceeds until their complete mineralization into inorganic products. The new prepared photocatalysts showed 2 to 3 fold increased activity compared to best commercially available photocatalysts Hombikat UV 100 and Degussa P25. The hydrogen peroxide oxidation over iron containing zeolites was demonstrated to completely purify cellulose factory discharge water from oligomers of cellulose. The developed in the laboratory air purifiers for cars and small rooms were started to be commercially produced in Luch Ltd utilizing catalyst IC-12-31.

Laboratory of Catalytic Processes in Fuel Cells

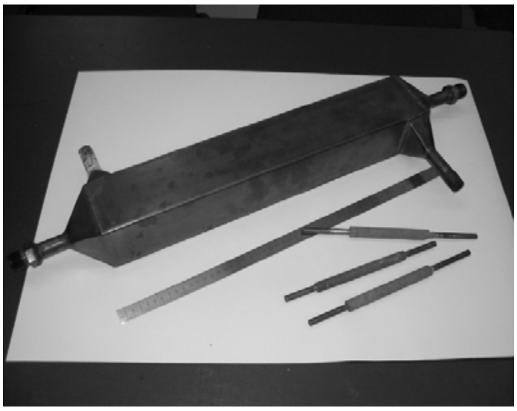
Head: Prof. Vladimir A. Sobyanin

- In hydrogen production from hydrocarbon fuels for proton-conducting polymer electrolyte fuel cells, the preferential CO oxidation reaction of carbon monoxide in the presence of hydrogen is used to decrease the CO concentration from 0.5–2 vol % to 10 ppm in the hydrogen-containing gas mixture. Pt- and Ru-based catalysts supported on γ-Al_2O_3, SiO_2 and graphite-like carbon material Sibunit were studied to determine dependence of the catalyst activity on the composition, preparation procedure and reaction conditions of the selective CO oxidation. The most active Pt/Sibunit catalysts were shown to provide a decrease in CO content in the hydrogen-containing mixtures to below 10 ppm at the temperature ranging from 150 to 180 °C and flow rate between 5000 and 20000 h^{-1}.

The proposed mechanism of CO oxidation over metal catalysts in the presence of hydrogen was based on data obtained by various physical methods. The results obtained were used to design a compact reactor with enhanced heat exchange to remove CO from hydrogen-containing gas to be fed to a fuel cell of 5 kWt capacity.



1vol. % CO+1.5 vol. % O_2 +10 vol.%H_2O + 20 vol.% CO_2 + 65 vol.% H_2 + He (balance) GHSV =12000 $ч^{-1}$



Reactor for hydrogen purification from CO

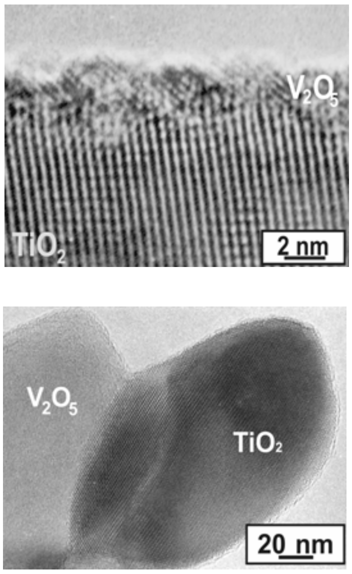
Laboratory of Catalysts Preparation

Head: Prof. Alexandra S. Ivanova

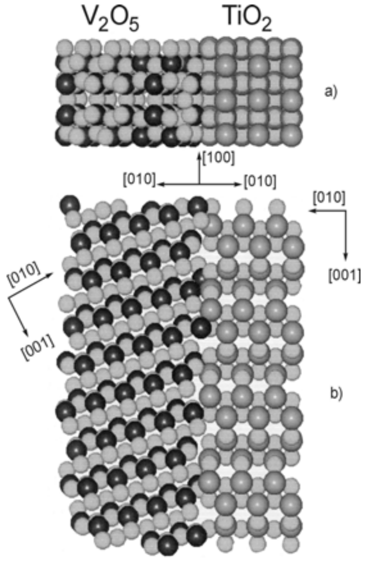
➢ 1. When disorderedly structured anatase is used as the initial compound, nanostructured V-Ti-O catalysts are formed which contain interphase boundaries built-up by V_2O_5 and TiO_2 (anatase) crystallites. HREM studies of the structural arrangement of the interphase boundaries in the catalysts comprising 5 to 50 wt % of V_2O_5 show their identical microstructures irrespectively of the vanadium loading: planes (310) of vanadium oxide are stacked with planes (110) of titanium dioxide, the angle between directions (001) of unit cells of TiO_2 and V_2O_5 being 17.4°. At the same time, the boundaries increase in length and number with an increase in the vanadium loading.

EPR and ^{51}V NMR spectroscopic studies reveal that vanadium ions are in the oxidation states V^{4+} and V^{5+} nearby the boundaries. V^{4+} ions are stabilized in the anatase structure to substitute for Ti^{4+} ions. From the Raman spectroscopic data, stabilization of vanadium ions along the interphase boundaries results in shortening the terminal V=O bond but lengthening the bridge V–O–Ti– bonds compared to those in the traditional V–Ti–O catalysts.

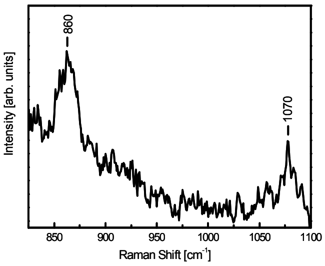
The prepared catalysts demonstrate a high activity and selectivity in a number of partial oxidation processes such as oxidation of β-picoline into nicotinic acid, formaldehyde into formic acid, *o*-xylene into phthalic anhydride and in some others, as well as in reduction of nitrogen oxide with ammonia.



Micrographs of V_2O_5/TiO_2 samples with 5 and 20 wt.% loading of V_2O_5



Schematic representation of the interface between V_2O_5 and TiO_2 viewed along [001] (a) and [100] (b) direction. Vanadium, titanium and oxygen atoms are depicted with black, dark gray and light gray balls, respectively.



Raman spectrum of the catalyst with interphase boundary: band at 860 см$^{-1}$ corresponds to V=O bond, band at 1070 см$^{-1}$ – bridge V-O-Ti bond

2. Characterization of structural features of phase-uniform aluminas formation prepared by thermal decomposition of aluminum hydroxides with structure of pseudoboehmite, boehmite, bayerite and gibbsite allowed the γ- and η-alumina microstructure to be established for the first time. The said spinel-structured oxides were shown to have different microstructural arrangement. γ-Al_2O_3 particles synthesized from boehmite are shaped as elongated (ca. 100 nm) fine monocrystalline plates with predominant {110} face. The principal feature of their microstructural arrangement is the presence of specific closed defects built-up by elongated dislocation walls that form due to coalescence of lattice vacancies during the structure evolution. In the η-Al_2O_3 particles, face {111} predominates; there are coherently stacked pronouncedly plate-like domains and a system of planar defects arranged in the (111) plane. The results obtained made it possible to explain the different strength and concentration distributions of the surface acid sites on the oxides.

Laboratory of Dehydrogenation
Head: Prof. Roman A. Buyanov

➢ • Technology for preparation of metal-fibrous carbon catalysts was developed. The feedstock and optimal conditions were chosen for the reaction of hydrocarbon decomposition to synthesize the catalysts. Experimental samples were synthesized and tested to demonstrate their high efficiency for purification of ethylene and butenes from mixtures of acetylene and butadiene, respectively;

• Facilities and new methods were developed for mechanochemical reactions, including catalytic reaction, conducted at high gas pressure and high temperatures. Unique inorganic and fine organic transformations are made possible. Mechanochemical reactions are achieved for the first time under these conditions;

• New theoretical knowledge about the state of solid catalysts in the course of mechanochemical activation (MCA) and after its termination is acquired. Thermodynamic analysis of systems under MCA conditions is achieved based on the knowledge to elucidate the influence of MCA on catalytic properties and to describe some specific features of mechanochemical synthesis of catalytic systems;

• The catalytic behavior of ammonia was established in the mechanochemical synthesis of magnesium-nickel intermetallide hydride at high hydrogen pressure;

• New catalytic system – 10 % VO_x/MgO – have been prepared by a modified aerogel procedure for one-step selective oxidative dehydrogenation of butane to butadiene in the presence of oxygen and iodine. Butadiene selectivity as high as 65-70 % has been achieved in temperature range 550-600 °C in the presence of small amounts of iodine at 75-80 % butane conversion.

Group of Synthesis of Nanodispersed Materials
Head: Prof. Oleg P. Krivoruchko

➢ • Among the materials synthesized for the first time are nanodispersed (d~1.5 nm) Co^{2+} hydroxide and Ni^{2+} hydroxide. In the former, cations are coordinated in unusual (for this type systems) way in oxygen tetrahedrons ($Co^{2+}{}_{Td}$), while the characteristic feature of the latter is the presence of absorption bands from spin-forbidden d-d transitions $Ni^{2+}{}_{Oh}$ in the DRS spectra. The unusual structural and electron properties of the synthesized hydroxides are mainly caused by size-induced effects of variously dispersed hydroxide particles. The results obtained show basically new prospects for synthesis of unique nanodispersed cobalt- and nickel-containing catalysts and high-tech materials for numerous application areas.

• Stabilization of Co^{2+} ions at the stage of synthesis of CoZSM-5 through interaction with extra-skeletal Al^{3+} atoms in the channels of HZSM-5 zeolite to form one-dimension (1-D) analogues of Co^{2+} oxo(hydroxo)aluminates containing $Co^{2+}{}_{Td}$ in a slightly distorted or ideal (depending on the preparation conditions) oxygen environment that is identified from the presence of an a.b. multiplet at 14500, 15000 and 16000 cm^{-1}.

• The fact of stabilization of Co^{2+} ions in the channels of HZSM-5 zeolites due to interaction with extra-skeletal aluminium is of importance for synthesis of other two-charge cation containing MZSM-5 zeoliets (M = Cu^{2+} etc.). The extra-skeletal aluminium is practically always available in HZSM-5 channels that makes it necessary to revise a number of already published conclusions regarding specific features of localization of M^{2+} ions in high-silica zeolites.

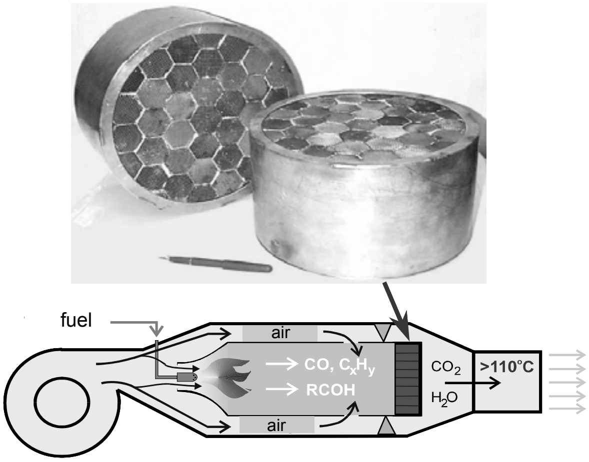
Laboratory of Environmental Catalysis
Head: Prof. Zinfer R. Ismagilov

➢ A universal heat generator *UCHG-0,34 "Pioneer"* with catalytic cleaning was developed by the Boreskov Institute of Catalysis in cooperation with the Siberian Agroindustrial House Co. and Engineering Vegetable-Growing Center "INTOS" for heating greenhouses, storage and productive facilities, as well as for emergency heating of municipal buildings.

The Pioneer operation is based on two-stage combustion of hydrocarbon fuel. The first stage is flame combustion of a liquid fuel; the formed flue gas is diluted with air and fed to a chamber with a catalytic cassette of honeycomb monolithic catalysts. The outlet hot air after the cassette meets completely the environmental standards for working areas. The generator operates in the automated mode.

Application of the Pioneer generator allows all the energy of fuel combustion to be almost totally transferred to heated air. The generator efficiency is over 99.5 % at complete fuel combustion. The heat generator has passed successful testing and pilot scale production of the generators *UCHG-0,34 "Pioneer"* has been organized.

Catalytic cassette with monolithic catalysts of honeycomb structure



Equivalence ratio oxygen/fuel (α)
at the first stage ≤ 1
to prevent NOx formation

Universal heat generator

UCHG-0,34 Pioneer

Laboratory of Catalysts for Deep Oxidation
Head: Prof. Vladislav A. Sadykov

- In collaboration with Lavrentiev Institute of Hydrodynamics and Laboratory of industrial catalytic processes of BIC, monolithic catalysts for the processes of hydrocarbons autothermal reforming and steam reforming based upon metallic and cermet substrates possessing a high electrical and thermal conductivity were elaborated. These catalysts allow to realize a fast start-up of reactors for the autothermal reforming of hydrocarbons as well as efficiently supply heat for the processes of endothermal steam and dry reforming.

Laboratory of Catalytic Conversion of Carbon Oxides
Head: Dr. Alexandr A. Khassin

- 1. Composition of Cu/ZnO and CuAl/ZnO methanol synthesis catalysts as prepared and hydrogen activated by *in situ* XRD and HR EM

The studies devoted to the reduction-reoxidation of $Cu_{0.08}Zn_{0.92}O$ and $Cu_{0.2}Zn_{0.7}Al_{0.1}O$ were continued. These two samples were shown to be solid solutions of copper and aluminium ions in imperfect zinc oxide. This type of solid solutions, being the precursors of active methanol synthesis catalysts, is formed through decomposition of the respective hydroxocarbonates at 570–770 K.

Based on known data and those obtained in last year the following interpretations may be proposed. During the formation of the CuZnO solid solutions, the foreign anions in anion-modified (am) oxides give rise to extended stacking faults of (002) ZnO lattice plane (esf). These are occupied by copper ions in the form of small clusters of the Cu^{+2}–O–Cu^{+2} type. The nearest oxygen environment of the copper ions in such a cluster is a distorted octahedron, exhibiting a nearly square plane. Aluminium ions dissolved in zinc oxide promote formation of these clusters, and prevent crystallization of a separate copper oxide phase with increasing copper ion concentration.

The main part of copper ions in the Cu^{+2}–O–Cu^{+2} clusters are reduced to Cu^{0} in hydrogen at 600 K. This metallic copper diffuses either to the external surface or to vacant inner holes of the *am*-ZnO crystal, and is observed as dark spots at electron micrographs (Fig. 1). At HRTEM micrograph (Fig. 2) it can be seen that these dark spot are made up of Moiré fringes parallel to ZnO (002) lattice plane with spacing of about 1 nm. This finding indicates a lattice coherence of the inclusion and the main crystal. Fourier pattern of the image of coherent inclusion (Fig. 3) shows the presence of two crystal lattices: ZnO and Cu^{0}. Copper atoms in the vacant holes form 2-3 nm clusters of the Cu^{0}–Cu^{0} type.

Copper metal particles on the surface of *am*-ZnO are reoxidized to Cu^{+2} at 600 K in a helium flow containing 0.05 vol. % oxygen (Fig. 4), and according to EM data they come back to the *esf*. The Cu^{0}–Cu^{0} clusters in the holes of *am*-ZnO are not reoxidized under these conditions. The same reduction-reoxidation processes were found to take place in the CuAl/ZnO catalyst.

The observed reduction-oxidation reversibility of the main part of the copper from the solid solution without any accompanying change in the ZnO structure provides evidence for the following mechanisms:

– Reduction of Cu^{+2} ions occurs through their substitution by protons in the ZnO structure: $H_2 \leftrightarrow 2H$; $Cu^{+2} + 2H = Cu^{0} + 2H^{+}$

– Oxidation occurs through the reaction of dissolved protons with O_2 from the gas phase, and electron transfer from the copper metal: $O_2 \leftrightarrow 2O$; $Cu^{0} + 2H^{+} + O = Cu^{+2} + H_2O$

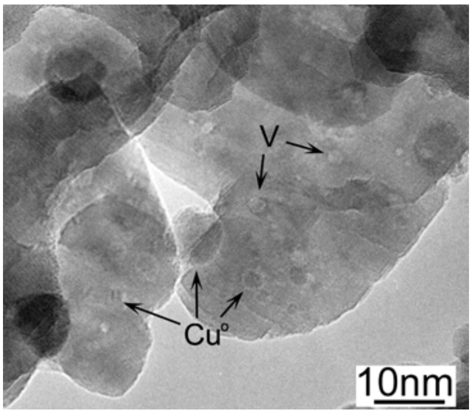


Fig. 1. Electron microscopy image of the $Cu_{0.08}Zn_{0.92}O$ sample reduced in H_2.

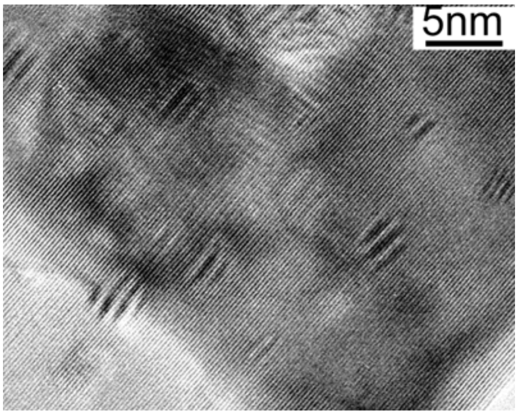


Fig. 2. High resolution electron microscopy image of $Cu_{0.08}Zn_{0.92}O$ reduced in H_2.

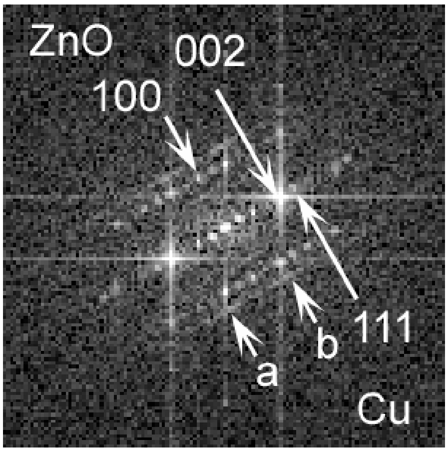


Fig. 3. Electron-diffraction $Cu_{0.08}Zn_{0.92}O$ reduced in H_2, indicating the coherence of the inclusion lattice and the main crystal

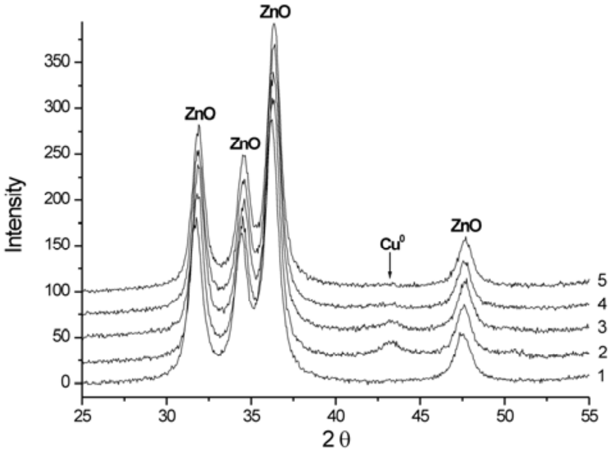


Fig. 4. *In situ* XRD patterns of $Cu_{0.08}Zn_{0.92}O$: (1) as prepared; (2) reduced in H_2; reoxidized in He + 0.05 vol% O_2 for (3) 1 h; (4) 2 h; (5) 3 h.

2. Membrane reactors for the Fischer-Tropsch synthesis

1. The studies of the Fischer-Tropsch synthesis in membrane reactors based on the **permeable composite monoliths (PCM)** was continued. PCM are characterized by:

- a high concentration of a catalytically active compound (0.9 – 1.1 g/cm^3);
- a high heat-conductivity (above 3 W/(m s));
- a high mechanical strength;
- a permeability, which is reasonable for Fischer-Tropsch synthesis ($10^{-14} – 5 \cdot 10^{-13}$ m^2);
- a well developed transport pore structure with the mean radius of ca. 2–5 μm and the concentration of ca $0.6–3 \cdot 10^9$ m^{-2}.

2. It is possible to prepare PCM membranes of different geometry (plate, hollow cylinder) and with different pore size distribution parameters. It has the significant impact to the catalytic properties of membrane. Two parameters of the pore structure are suggested to account for the difference in membrane performance. The width of the transport pores distribution by size is responsible for the extent of gas flow bypass and for the extensiveness of stagnation zones inside the membrane. The inhomogeneity of the distribution decreases specific activity of the membrane. On the other hand, the concentration of transport pores (i.e. the mean distance between two adjacent transport pores) is related to the magnitude of the diffusion constrains. This plays the important role for the selectivity of the process with respect to higher hydrocarbons. The data on the selectivity with respect to olefins are accounted for by both: the remoteness of transport pores from each other (hindering the olefin escape processes) and the width of transport pores distribution (extending the stagnation zones). It is noteworthy that the study seems to give another argument pro the hypothesis that olefins are the primary product of the Fischer-Tropsch synthesis, while all the paraffins (except methane) are the secondary products of olefins hydrogenation.

3. The geometry of membrane is shown to affect a lot its performance in the Fischer Tropsch synthesis. The positive curvature of membrane promotes the productivity of membrane and its selectivity towards higher hydrocarbons. On the other hand it promotes also the process of olefins hydrogenation to paraffins. For the latter process, the study suggests the simple explanation based on the effect of the membrane curvature on the wetting extent profile along the membrane.

4. The obtained results prove that the membrane reactors are effective for the Fischer-Tropsch synthesis and that the performance of the PCM Fischer-Tropsch synthesis can be controlled at the early stage of the membrane preparation.

3. *Ni-Si-containing catalysts for methane steam reforming*

The activity of Ni-Mg amesites in methane decomposition were studied by *in situ* thermogravimety. The process of methane decomposition was shown to proceed consequently in kinetic, internal diffusion, and external kinetic regions as the filamentous carbon is accumulated in the sample. The activation energy of the methane decomposition in the external kinetic region was measured as 190±5 kJ/mole, which is in a good agreement with the literature data on ethane decomposition. This allows to suppose that the reaction rate is controlled by the C—H bond cleavage of the adsorbed methane molecule. For reference sample Ni/MgO, the preexponential factor is above 10^{13} s^{-1}, while Ni-Mg amesite are much less active ($k_0 = 10^{-12}$ s^{-1}). The amount of the accumulated carbon at 790 K till the complete deactivation of the catalyst related to the amount of metallic Ni is manyfold lower for Ni-Mg amesites (less than 60), than for Ni/MgO (350–380). These observations prove the earlier made conclusions on the high stability of Ni-Mg amesites in the processes of methane conversion to the synthesis gas.

Group of Catalytic Synthesis of Oxygen-Containing Compounds

Head: Dr. Galina G. Volkova

- Solids known as superacids: $Rh/Cs_xH_{3-x}PW_{12}O_{40}$, $Rh/SO_4/ZrO_2$, $Rh/WO_x/ZrO_2$ were studied as catalysts for halide-free carbonylation of dimethyl ether to methyl acetate:

$$CH_3\text{-}O\text{-}CH_3 + CO \rightarrow CH_3\text{-}CO\text{-}O\text{-}CH_3$$

Samples	Rate 10^{-8} mol $g^{-1}s^{-1}$	Selectivity, %	Bronsted acid sites		Lewis acid sites
			N, µmol g^{-1}	PA, kJ mol^{-1}	N, µmol g^{-1}
$Rh/Cs_{1.5}H_{1.5}PW_{12}O_{40}$	45	94	128	1120	32
$Rh/SO_4/ZrO_2$	3	10	38	1160	105
$Rh/WO_x/ZrO_2$	6	50	38	1180	37

The nature of active species for activation of C-O bond in dimethyl ether molecule was revealed: strong Bronsted acid sites with strength PA = 1120 kJ mol^{-1} and density ~120 µmol g^{-1} are responsible for activation of C-O bond and halide-free DME carbonylation over $Rh/Cs_{1.5}H_{1.5}PW_{12}O_{40}$ catalyst. At the same time Lewis acid sites induced the cracking of DME molecules that led to very poor activity and selectivity of $Rh/SO_4/ZrO_2$ catalyst.

Group of Catalytic Conversion of Sulfur-Containing Compounds
Head: Prof. Anna V. Mashkina

- Regularities of condensation of alkylmercaptans similar to those containing in natural gas were studied in the presence of an improved catalyst ICT-37-6. Specific features of the process depending on the structure of initial mercaptan were revealed. The process conditions for synthesis of dialkyl sulfides from lower alkylmercaptanes were specifies.

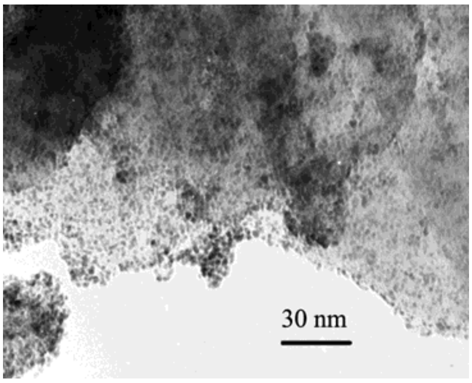
Laboratory of Sulfide Catalysts
Head: Prof. Anatolii N. Startsev

- A novel catalytic reaction of low temperature decomposition of hydrogen sulfide into hydrogen and elemental sulfur is discovered. This reaction is carried out under conditions of coupling of conjugated chemisorption and catalysis with 100 % conversion and selectivity.

Group of Heterogeneous Catalysts on the Basis of Noble Metals
Head: Anatolii V. Romanenko

- In connection with rough development of fuel elements production, the interest of obtaining of highly dispersed catalysts M/C with a high metal content, of 15 to 40 wt %, has sharply increased. It turned out, that the synthesis of such catalysts requires searching of the new approaches to metal supporting.

In the group the methods of synthesis are developed and highly dispersed samples of platinum and platinum-ruthenium electrocatalysts with a high content of Pt and Ru supported on carbon support with a low surface area, of 10 to 100 m^2/g, are prepared. Figure represents the HREM micrograph of catalyst 20 % (Pt-Ru)/C (Pt\Ru = 1:1) prepared on the support of Sibunit type with BET surface area of 60 m^2/g.



Group of Catalysts and Processes Based on HeteropolyAcids
Head: Prof. Klavdii I. Matveev

- The composition of a new patent able catalyst Pd+HPA$_x$ to be used in the MEK process in the presence of limit admissible concentrations (LAC) of products of special steels corrosion ([LAC] ≤ 0.1 M) was developed to substitute for the Pd+HPA catalyst which is only appropriate for non-corroding titanium facilities.

Methods for quantitative chromatographic analysis of the MEK process feedstocks (*n*-butens) and the oxidation products were developed.

Methods were developed for analytic control of the concentrations of palladium and its stabilizator Pc in the Pd+HPA$_x$ catalyst for the MEK process.

Group of Metal Complex Catalysis

Head: Dr. Nina I. Kuznetsova

- Gas-phase hydroxylation of benzene with a mixture of O_2 and H_2 was revealed to proceed on bi-component silica supported catalysts consisted of platinum metals and heteropoly compounds. Productivity of the catalysts in gas-phase hydroxylation of benzene is a function of a nature of platinum metals and heteropoly compounds, the active components loading, surface area of the silica support and temperature of the process. Productivity of the catalysts of optimal composition at appropriate temperature amounts to 400 mol of phenol per 1 g-atom of Pd or Pt per 1 hour, that is several times higher than one of the literature known catalysts. It was found the catalytic properties of the samples to be subjected to some modification during catalysis or prior to catalysis by means of wet treatment.

Activity of the catalysts is associated with zones of contact between platinum metal and heteropoly compound.

The active species of the catalysts were simulated by bulky samples of the appropriate composition. Interaction of Pd(II), Rh(III), Ru(III), Ir(III) chlorides and phosphomolybdic heteropolyacid was studied by means of IR, UV spectroscopy and XPS, providing typical conditions of the catalysts synthesis. It was established formation of mixed-valent associates $(Pt^{0,II}{}_nCl_mO_xH_y)\cdot(PMo^{VI,V}{}_{12}O_{40})$ $(n = 0{,}5 - 1,\ m = 0{,}2 - 1,\ x = 1 - 3)$, which represent finely dispersed platinum species stabilized by the heteropoly anions.

Center for Catalysts Characterization and Testing

Head: Prof. Bair S. Bal'zhinimaev

- The modelling of self-oscillations and surface autowaves in CO oxidation reaction over Pd(110) has been carried out by means of the Monte-Carlo technique. The synchronous oscillations of the reaction rate and surface coverages are exhibited within the range of the suggested model parameters (under the conditions very close to the experimental observations). The role of adsorbed CO diffusion as a synchronisation factor between the separate oscillating surfaces in CO oxidation reaction has been examined. As a result of the chosen simulation strategy the spiral waves of adsorbed species on the palladium surface (imagined as a set of independent Pd(110) planes communicating by surface diffusion) have been observed. It has been established that the adsorbed CO diffusion anisotropy does not influence the oscillation kinetics (period and amplitude of oscillations do not change) but leads to the appearance of the propagating reaction fronts on the palladium surface elliptically stretched along the $[1\bar{1}0]$ direction in close agreement with the known experimental data (photoemission electron microscopy – PEEM).

Laboratory of Catalytic Activity Testing
Head: Dr. Nikolai N. Bobrov

- A unique BI-SORBchemo instrument is designed for measuring surface areas of supported metals by the method of oxygen titration. The BI-SORBchemo instrument is superior to all the analogues due to the application of a digital pulse system for feeding sorbate samples to the material under studies that provides an increase in the dynamic range by two orders of magnitude and in the measurement accuracy and a comfortable handling.

Laboratory of Industrial Catalytic Processes
Head: Dr. Il'ya A. Zolotarskii

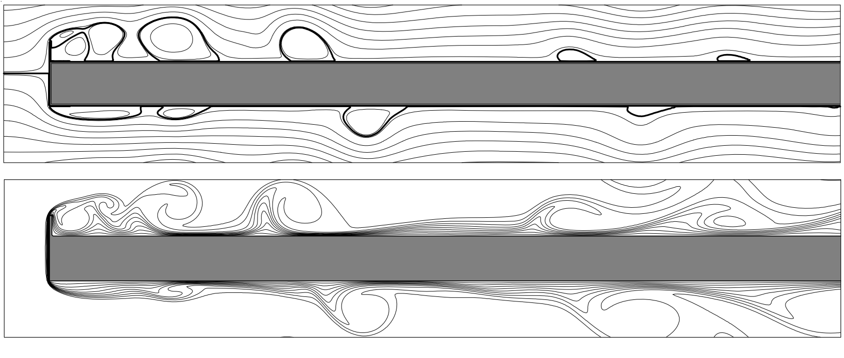
- ***Development and CFD-study of methods of mass transfer intensification in honeycomb catalyst channels***

Computational fluid dynamics is a powerful tool for solution of wide spectrum of chemical technology and catalysis problems. Their applying permit to find out, that at certain ad hoc organized conditions in honeycomb channels the pulsatory vortex-shedding regimes are realized. In these regimes a considerable increase of mass transfer rate takes place. Numerical experiments show 1.5-2.0 fold conversion rise. The other aspects, which are of fundamental importance for realization of catalytic processes in honeycomb catalysts, have been found during the study. Among them – extreme non-monotony of longitudinal distribution of local mass transfer rate. This effect is caused by wall thickness.

Four methods of flow turbulization in channels were approved numerically:

- inlet burrs placing;
- skew flow feed;
- walls perforation;
- monolith «screening».

Flow conditions correspond to those in the ammonia oxidation reactor of high pressure nitric acid plants. Thick-walled iron-oxide honeycombs with a square channels are used in these reactors along with platinoid gauze pad. Theirs real geometry were reduced to infinite two-dimensional flat-periodic system "thick plate – slit channel".

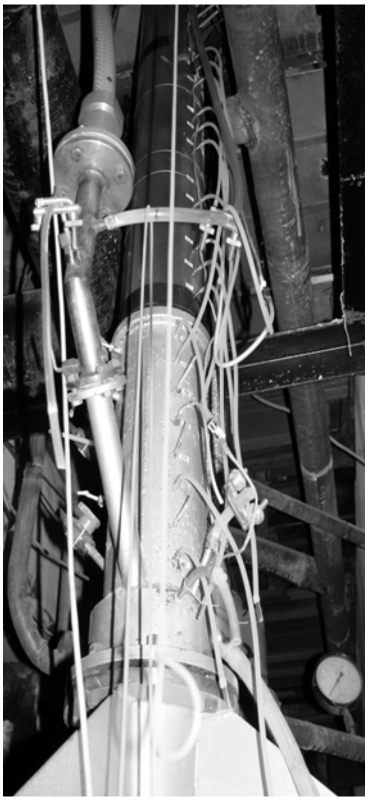


Momentary flow pattern (on top) and concentration field (below) in a burred channel. Gas moves from left to right. The burr is situated on the left upper plate edge.

Fluidized bed studies

Development of reliable hydrodynamics model of turbulent fluidized bed reactor is an important task of chemical reactor design and modeling. To perform an experimental investigation of hydrodynamics properties of turbulent fluidized beds two cold flow models of 0.15 and 0.7 m ID are constructed. The first model is of pilot scale size, and the last one is of industrial scale. Using different fluidizable media the following methods of studying of fluidized bed properties are developed:

- Measurements of bed expansion and dense-phase gas hold-up using pressure transducers technique
- Determination of the transition from bubbling to turbulent fluidization by using in-bed pressure fluctuations measurements
- Investigation of radial fluidized bed structure and measurements of the interphase mass transfer coefficients by using inert gas tracer technique



Cold flow model of 0.15 m ID

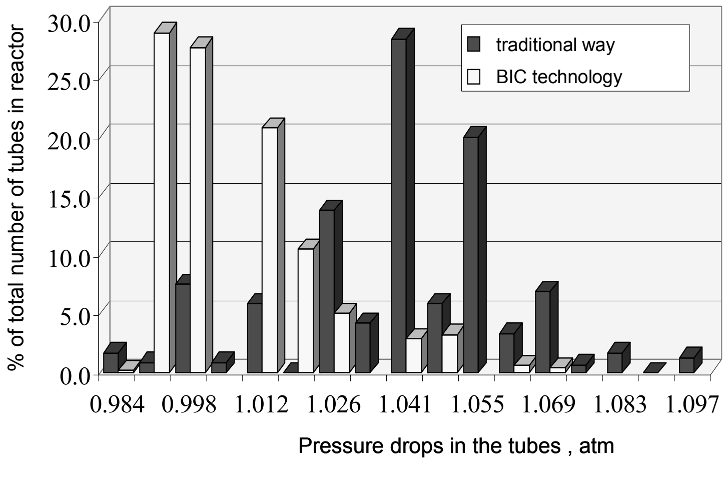
Cold flow model of 0.7 m ID

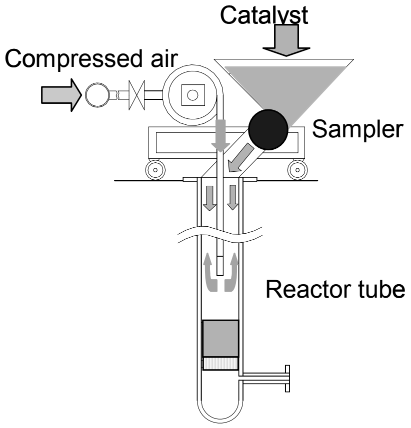
Laboratory of Unsteady-State Catalytic Methods for Gas Purification

Head: Prof. Alexander S. Noskov

➢ Theoretical and experimental studies were focused on development of the method for loading of granulated catalysts in tube reactors. Mathematical modeling has been used to study various manners of packing of grain bed structures in individual tubes of the catalytic reactor. It was demonstrated by calculations that the maximal bed uniformity along the tube radius is achieved at the successive packing to the minimal potential energy sites. In order to make the catalyst particles packed in these sites, the uniform distribution of the catalyst particles along the tube radius and their falling from equal height into the packed bed should be provided. As a result, the granules are predominantly packed into the minimal potential energy sites. If all the particles are made falling from the same height, a uniform density of the grain bed and, correspondingly, equal pressure drop is provided in all the tubes of the reactor.

To create technical facilities for loading in tube reactors, the method of aerodynamic deceleration of falling particles was developed using the countercurrent air flow that prevents destruction of the free falling catalyst particles in the tube. Requirements to parameters of the decelerating air flow resulted from the necessity of the rate of particle falling in the tube equal to the free falling rate from a given (1 to 1.5 m) height. The air flow parameters were determined for complex-shaped particles using methods of computational hydrodynamics to be checked experimentally.





Based on the results obtained, an automated loading facility was designed and assembled. It was first used to load in the industrial tube reactor for steam conversion of natural gas at Methanol Co. (Tomsk). A catalyst in amount of 53 t was loaded into the reactor consisting of 496 tubes of 12 m height. Deviations of pressure drops in the tubes fell into the range of ±3 to ±4.5 from the average. The results obtained are the best worldwide for reactors of steam conversion of natural gas

Laboratory of Catalytic Conversion of Solid Fuels and Wastes
Head: Dr. Alexander D. Simonov

- Technical data for designing an industrial catalytic heat generator operating with solid and liquid fuels were developed on the basis of analysis of long-term operation of industrial and demonstration catalytic heat generators KTU-02. Technical data for manufacturing of a prototype model of a serial solid- and liquid-fueled heat generator is prepared at the Novosibirsk Plant of Chemical Concentrates.

Bench testing was carried out on combustion of liquid and solid fuels in a fluidized inert bed in the presence of fixed catalytic packing in a reactor of 170 mm in diameter. The test data supported earlier results obtained with a reactor of 40 mm in diameter, i.e. scaling-up does not considerably affect the process of fuel combustion in a fluidized inert bed in the presence of a fixed catalytic packing.

Group of Catalytic Technologies for Carbon Material Synthesis
Head: Dr. Dmitrii G. Kuvshinov

- A new kinetic model corrected for the catalyst deactivation is proposed for the atmospheric-pressure process of NFC formation from a mixture of $CH_4 – H_2$ over a high-nickel catalyst. The model describes better way the related experimental data and indicates the asymptotic decrease in the catalyst activity as a function of time.

The developed mathematical modeling methods provide calculations and analysis on operation of both batch and flow reactors for catalytic synthesis of nanofibrous carbon materials from methane and natural gas.

Group of Mathematical Methods for Catalytic and Adsorption Processes Modeling
Head: Dr. Natalia A. Chumakova

- A detailed study of two- and three-variable mathematical models of a heterogeneous catalytic hydrogen oxidation over metallic catalyst is performed. At the centre of attention is the phenomenon of weakly stable dynamics, a type of complex irregular behavior frequently encountered in oscillating chemical reactions. One of the most important properties of the weakly stable dynamics is “a sensitive dependence on the initial conditions”. The analysis of a global error in long-term numerical integration of dynamical system shows that a high-sensitive dependence on the initial conditions appears in the considered three-variable system with fast, intermediate and slow variables due to existence of the “Canard cycles” which occur close to the Hopf bifurcation in the one-parameter family of two-variable subsystems. Moreover, a key feature of the weakly stable dynamics appearance can be successive period doubling bifurcations through which the system behavior becomes progressively more complex until the attractor appears. The results obtained are of interest for mathematical modeling of different heterogeneous catalytic reactions with complex dynamics if the corresponding model has the hierarchy of characteristic time scales.

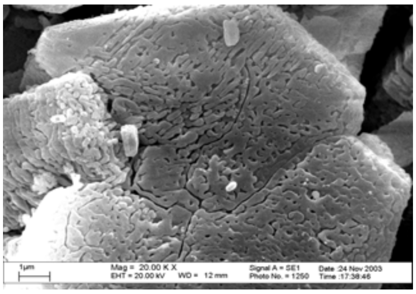
Laboratory of Catalytic Hydrocarbon Conversion

Head: Prof. Gennadii V. Echevskii

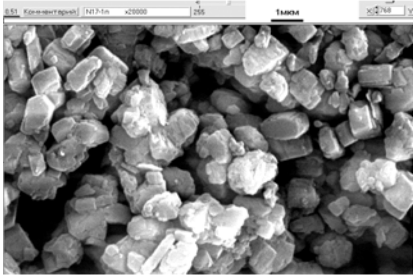
➢ The traditional approach to synthesis of nanosized crystals is based on pre-ageing of gels, varying compositions of gels and conditions of ageing or crystallization of mixtures; therefore the syntheses takes long time (months) and isolation of the target solid is very difficult. The new method allows the residual chemical reactivity of microspherical or monolith alumina supports to be used for synthesis of nanosized zeolite crystals with various morphologies and chemical composition on the outer surface of prepared supports. Synthesis of these materials takes the same time as the synthesis of micron sized zeolite crystals but causes no problem to isolate the solid product. The nanoscale size of the synthesized zeolite crystals is identified using adsorption and HREM techniques. The size and morphology of the grown crystals is determined by the polymorphous modification of the alumina support used. Their chemical composition depends both on the composition of the initial reaction gel and on the chemical activity of the support. XRD studies indicate formation of pure zeolite phases such as ZSM-5 or Beta-zeolite. Due to practically no diffusion limitations inside the zeolite channels, the synthesized systems reveal much higher (by an order of magnitude) activity and considerably different selectivity than conventional micron-size zeolite systems; this is supported, for example, by test data on conversion of methanol into hydrocarbons.

The proposed approach allows a variety of nanosize porous crystal materials to be synthesized on the outer surface of supports of various chemical natures and innovative composite materials with unknown properties to be created.

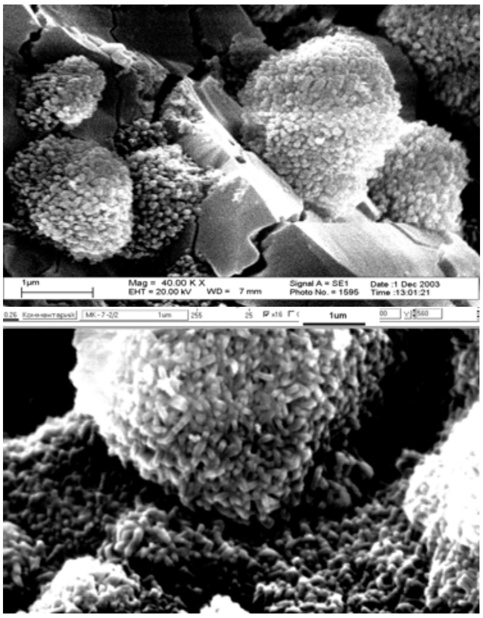
Initial support based on α- Al_2O_3



Dimensions and morphology of zeolite synthesized by traditional method (without support)



Dimensions and morphology of zeolite grown on the outer surface of microspherical supports



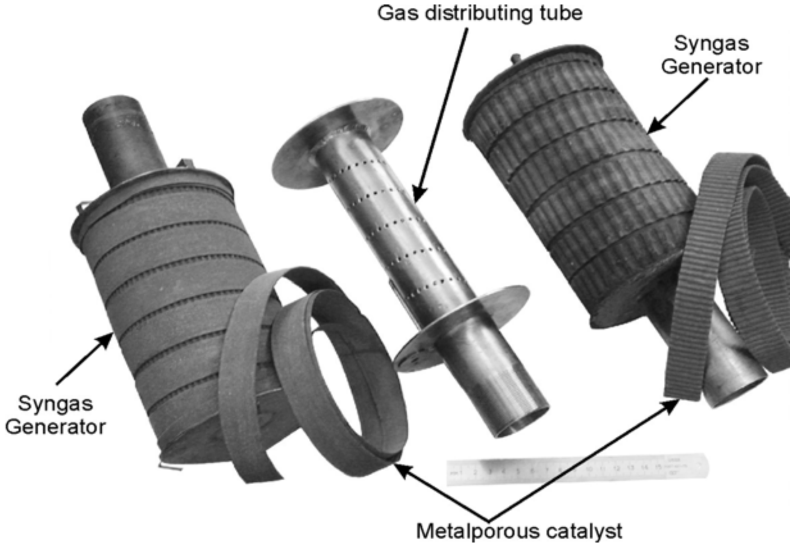
Laboratory of Multiphase Processes Modelling

Head: Prof. Valerii A. Kirillov

➢ The rapid increase in number of motor vehicles causes greater amount of harmful exhausts to the atmosphere. This becomes the main source of environmental pollution in many large cities worldwide. The traditional method for detoxication of motor exhausts it to use expensive catalytic neutralizators to provide reburning of CO and minimization of NO_x concentrations in the exhaust gases. Other speaking, the currently used methods for reduction of toxic exhausts are aimed at treatment of the consequence of principal shortcomings of fuel combustion in the engines. An alternative way to resolve the problem is on-board production of synthesis gas from the hydrocarbon fuel during the engine operation and application of this gas as an additive to the fuel.

A syn-gas generator for on-board conversion of hydrocarbon fuels is designed. It is a kind of radial reactor consisting of a one end plugged gas-distribution perforated tube and a catalyst bed. The catalyst bed is assembled from gas-permeable flat and corrugated catalyst strips that are reeled round the gas-distribution tube and sintered with it. The strips are arranged so as to form a porous structure consisting of large transport pores – channels (corrugations) and fine pores (catalyst porosity).

In 2001, bench testing of a VAZ-2111 gasoline engine equipped with an experimental syn-gas generator was carried out in Toliatti. The achieved economy in gasoline consumption with addition of syn-gas was 42 % at idle speed and 24 % in operation. At the same time a considerable decrease (10 to 15 times) in the amount of exhausted CO and NO_x was observed with syn-gas additives, the amount of CO being no more than 0.2 % in exhaust gases. Identical results were obtained during short-term testing of a M406 engine (Volga car) in 2003 in Moscow. The engine was made operating with a lean mixture of natural gas and synthesis gas. The experiments demonstrated ca. 20–30 times decrease in the exhausted amount of nitrogen and carbon oxides (ca. 300–400 ppm of carbon oxides and 20–30 ppm of nitrogen oxides) at a lower (by ca. 20 %) consumption of natural gas. Thus, application of synthesis gas as an additive to liquid and gaseous fuels for internal combustion engines provides a considerable decrease in the concentrations of carbon and nitrogen oxides in automotive exhaust gases and 20–25 % decrease in the consumption of hydrocarbon fuel due to application of lean fuel mixtures allowing the stable engine operation.



Laboratory of Dynamics of Catalytic Processes

Head: Dr. Andrey N. Zagoruiko

- 1. Industrial installation for selective catalytic H_2S oxidation for cleanup of Claus unit tail gases was constructed at Omsk Refinery (Omsk, Russia). Installation maximum tail gas capacity is equal to 10 thousands m^3/hour. Both process technology and catalyst were developed by the laboratory. Start-up works at the installation are in progress.

2. The pilot plant construction and pilot tests of Pt-based glass-fiber catalyst were performed at Byisk Oleum Plant (Byisk, Altai Region, Russia). The tests made in media of real gases of sulfuric acid production showed high activity and high operation stability of the catalyst. Unique experimental data on mass exchange in layers of fiber catalyst were obtained. On the base of achieved results the wide scale implementation of glass-fiber catalysts at sulfuric acid plants is planned.

3. Theoretical basis was developed for nonstationary catalytic process with separate reagents feeding for a complex system of selective exothermic reactions in a “reversed” heat front. In this case the heat wave is moving upstream the reaction mixture flow due to heat conductivity of the fixed adiabatic catalyst bed. Numerical simulation of model problem showed that such regime may provide significant increase of reaction selectivity and aim product yield, moreover, the observed value of maximum process temperature is kept at relatively low level and thus the overheating of the catalyst is provided. Described approach may be applied to reactions of selective oxidation of hydrocarbons, as well as to variety of complex exothermic reaction systems

Laboratory of Nucleation Processes

Head: Prof. Dr. Mikhail P. Anisimov

- Diagrams of the dynamic phase equilibria are substantiated and introduced as a new class of diagrams. Using of the dynamic phase equilibria diagram conception originates the scientific explanation of the empirically recognized effect of the component separation efficiency growth at the fractional distillation (for example, petroleum) with aerosol formation. New class of diagram yields the goal-seeking optimization of the fractional distillation conditions to reach the efficiency maximum of the component separation. That result has impact to the broad spectrum of technologies based on the component fractional distillation.

The computer algorithm for semiempirical construction of nucleation rate surfaces is created. The nucleation rate surface for water vapor nucleation is designed for the temperature span from absolute zero to critical one.

The first stage of the flow diffusion chamber having the record available total pressure value up to 120 Atm for the nucleation system has been drove. The chamber has yielded for one mixture to get the nucleation rate growth and drop against the total pressure of the nucleation n-pentanol–helium system for the first time in the world. It makes more accurate the topology of nucleation rate surface of system under investigation and give rise to conclusion that the resulting positive or negative effect is a matter of trajectory in the space of the system parameters. Result has impact for development of the topology comprehension for nucleation rate surfaces.

State of art review of the nucleation theory and experiment is done. Correlations for Vapor Nucleating Critical Embryo Parameters are established using the published data.

St. Petersburg Division of the Boreskov Institute of Catalysis
Head: Prof. Sergey S. Ivanchev

➢ 1. The general possibility and optimum conditions for supporting of bis(imino)pyridine-iron chloride and diimine-nickel bromide complexes onto silica "Davison 952" are determined. The ligands containing cycloaliphatic, particularly cyclohexyl substituents in the aryl ring are determined to provide the highest ethylene polymerization activity for $FeCl_2$- and $NiBr_2$-based catalyst systems. Three variants of the recipes and supporting conditions are suggested.

The application of catalyst mixtures comprising Ni-bis-imines and Fe-bis(imino)pyridines with MAO is studied for homogeneous polymerization. The process kinetics is found to be non-additive relating to the contributions of the mixture components. A possibility to provide the control over the polymer molecular weight distribution is also shown using this approach.

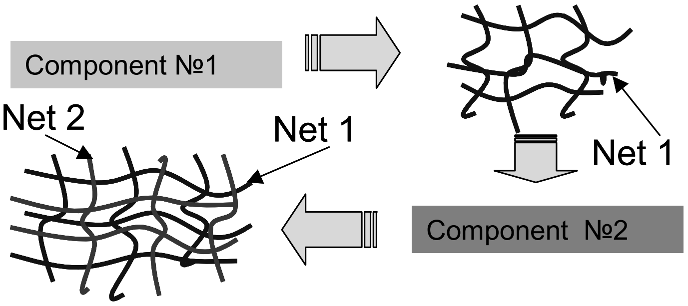
Studies of the catalyst activity of various phenoxy-imine derivatives for ethylene polymerization are started. A possibility for performing "living" polymerization using a phenoxy-imine derivative with a relatively simple structure bis[N-(3-tert-butylsalycilidene) anilinato]$TiCl_2$ in combination with methylaluminoxane at 30-50 °C is revealed for the first time.

2. A fundamentally new method for cationic hollow particle latex preparation is developed. The method comprises three general stages:

- vinyl benzylchloride (VBC) (co)polymer latex preparation,
- preparation of core-shell particle latex with VBC (co)polymer core and poly(methyl methacrylate) shell,
- amination of VBC (co)polymer followed by core swelling, shell expansion and hollow formation.

The use of this reaction sequence for hollow particle latex preparation was pioneered.

3. A unique very simple method is developed for preparation of extended-wear contact lenses. The method is based on synthesis of successive interpenetrating nets (IPN). The first stage is the synthesis of a silicone net via interaction of hydride- and vinyl-containing oligodimethylsiloxanes. At the second stage, saturation of the synthesized cross-linked polydimethylsiloxane with a solution containing hydrophilic monomers (N-vinylpyrrolidone or limethylacrylamide), cross-linked co-monomer and photoinitiator is followed by photopolymerization. The created material possesses a set of non-compatible properties required for manufacturing of extended-wear soft contact lenses.



The proposed method for synthesis of the material has been implemented by the technology of reactive molding that has allowed a SCL prototype to be created. The material and SCL have been subjected to medical and biological testing to establish that they meet world standards in physicochemical properties and such criteria as toxicoallergic reactions, hypoxic aftereffects and morphological changes of cornea.

Scientific and Engineering Center “ZEOSIT”

Head: Prof. Kazimira G. Ione

- New bifunctional catalysts were proposed for synthesis of liquid hydrocarbon from syngas; their catalytic properties were characterized in transformation of CO and H_2. The developed catalysts were compared to the traditional non-selective Fisher-Tropsch catalysts (catalyst F-T, see Fig. 1); they were shown to allow one-stage selective synthesis of high-octane gasoline fraction (catalyst BFC-2) or a diesel fraction with a high content of iso-paraffins (catalyst BFC-1). It is seen in Fig. 2 that the developed bifunctional catalysts are very active to isomerization: the iso-CH/h-CH ratio is 7 to 14 in the gasoline fraction obtained with BFC-2 and 1.5 to 2 in the diesel fraction over BFC-1. The properties of the BFC-1 catalyst and the process parameters can be varied to allow the iso-paraffin content to be controlled, the cetane number and freezing point to be selectively influenced in the synthesized diesel fraction. The results obtained are important to petrochemical practice in order to establish industrial production of motor fuels from alternative raw materials (natural gas, coal, bioorganic wastes etc.).

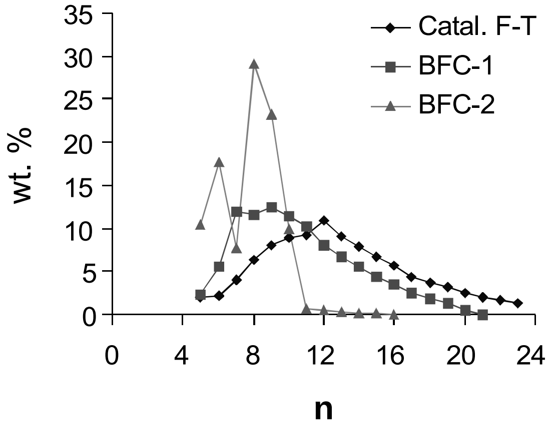


Fig. 1 Distribution of C_{5+} hydrocarbons in dependence on carbon numbers (n) in fractions, obtained in the process of syngas conversion over bifunctional (BFC-1, BFC-2) and Fischer-Tropsch (F-T) catalysts

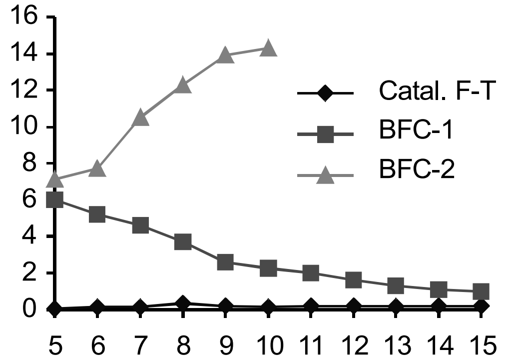


Fig. 2 Ratio between iso (i-CH) and normal (n-CH) hydrocarbons in dependence on carbon numbers (n) in C_{5+} fractions, obtained in the process of syngas conversion over bifunctional (BFC-1, BFC-2) and Fischer-Tropsch (F-T) catalysts

Omsk Division of the Boreskov Institute of Catalysis
Head: Prof. Vladimir A. Likholobov

- 1. *Development and improvement of catalysts for cracking of heavy residual stock*

An octane-enhancing additive to cracking catalysts is developed using ZSM-5 zeolite and a matrix based on reprecipitated aluminium hydroxide and bentonitic clay. Test data for catalyst CMZ-99, both individual and containing the additive, are shown in the Table. Application of the octane-enhancing additive allows the octane number of cracking gasoline to be enhanced and the yield of feedstock for alkylation (butylenes and isobutene) to be increased.

Table

Extraction of cracking products	*Additive-free*	*With additive*
Yield of gasoline, wt %	59.0	58.5
Selectivity for gasoline	82.4	82.1
Octane number of the gasoline (MON)	80.5	81.5
Product concentration in the produced gas, wt %:		
Butylenes	19.0	21.5
Isobytane	20.0	28.9
Isobutylene	3.0	3.3

A semicommercial batch (700 kg) of the octane-enhancing ZSM-5 based additive was produced at Omsk Refinery – Sibneft Co. Large-scale testing of the additive in catalytic cracking facilities demonstrated again its high efficiency. Even though the additive amount was no more than 0.3% in the cracking catalyst, MON was increased by 0.5 and the stock extraction for the process of alkylation was made higher.

2. *Development of catalysts of new generation and modernization of reforming technology for production of high-octane gasolines*

Two types of catalysts, PR-61 and PR-71, are developed for reforming of oil hydrocarbons.

The new PR catalysts are even more active than the commercial catalyst PR-51 and, that is of particular importance, provide the selectivity to paraffin aromatization as high as 60% to enable boosting the efficiency of reforming units in Russia in order to arrange production of gasolines with octane number 98 – 100 without considerable investments.

Both of the new catalysts were recommended for practical applications. The technical state of industrial reforming facilities was inspected at the Ryazan Refinery Co. Technical data for the installation reconstruction in order to make it operating in a more severe mode for production of reformate with RON = 98 – 100 using the new commercial catalyst PR-71.

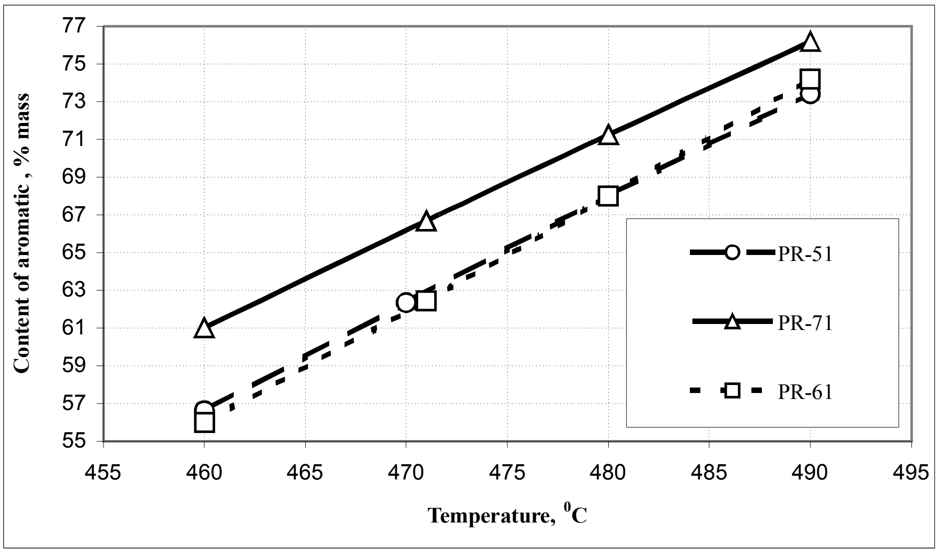


Fig. 1. The content of aromatic hydrocarbons in reformate as a function of process temperature

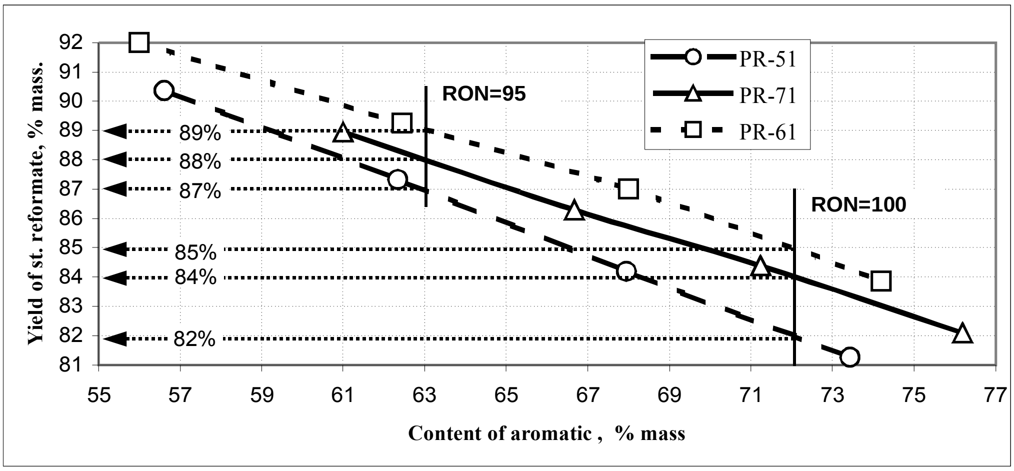


Fig. 2. Dependence of the yield of stable reformate on the content of aromatic hydrocarbons

RESEARCH ACTIVITY

Quantum-Chemical Studies

SEMI-EMPIRICAL CALCULATIONS ON THE STABILITY AND REACTIVITY OF NHX SPECIES ON METAL SURFACES

A.R. Cholach, N.N. Bulgakov, B.E. Nieuwenhuys*
(*Leiden Institute of Chemistry, Leiden,
The Netherlands)

Catal. Lett., 86 (1) (2003) pp. 9–16.

The semi-empirical Method of Interacting Bonds was used to elucidate the mechanism of oscillation phenomena in the NO+H_2 reaction on metal surfaces. Basic single-crystal planes of Pt, Rh, Ir, Fe, Ru, and Re were examined with respect to the stability of adsorbed NH_n species (n = 0, 1, 2, 3); to the reactivity of NH_n (n = 0, 1, 2) species toward adsorbed hydrogen atoms; and to the possibility of combination reactions between two NH or two NH_2 species resulting in the formation of gaseous N_2 molecules. All studied surfaces were found to form readily stable NH species. The principal difference between Pt, Rh, and Ir single-crystal planes exhibiting reaction rate oscillations, and Fe, Ru, and Re surfaces, which do not show an oscillatory behavior, is that the combination reaction of NH species can easily proceed in the former case, whereas this reaction is not allowed thermodynamically in the latter. This result is consistent with an earlier suggested model that attributes the oscillatory surface wave propagation to the intermediate formation of NH species.

Stable NH_2 species can be formed on Ru, Re, and Fe surfaces, whereas the noble metal surfaces of Pt, Rh, and Ir can only form weakly stable NH_2 species at the very edge of their existence region. The combination reaction between two NH_2 species is endothermic in all cases.

THE ROLE OF NH_n SPECIES IN OSCILLATION PHENOMENA IN THE NO + H_2 REACTION ON NOBLE METAL SURFACES: SEMI-EMPIRICAL CALCULATIONS

A.R. Cholach, N.N. Bulgakov, B.E. Nieuwenhuys*
(*Leiden Institute of Chemistry, Leiden,
The Netherlands)

Chem. Sustain. Devel., 11(1) (2003) pp. 47–54.

The semi-empirical Method of Interacting Bonds was used in the present work to clarify the mechanism of the title process. Various single crystal planes of Pt, Rh, Ir, Fe, and Re were examined with respect to the stability of the adsorbed NH_n species (n = 0, 1, 2, 3); to the reactivity of NH_n (n = 0, 1, 2) species towards adsorbed hydrogen atoms; and to the possibility of proceeding the combination reactions between two NH or two NH_2 particles resulting in the formation of gaseous H_2 and N_2 molecules. All the surfaces studied were found to form readily the stable NH species. The principal difference between Pt, Rh, Ir single crystal planes, on which the reaction exhibits rate oscillations, and Fe, Re surfaces, which do not show an oscillatory behaviour, is that the combination reaction of NH species can easily proceed in the former case, but this reaction is not allowed thermodynamically on the latter surfaces. This result is consistent with an earlier suggested mechanism for the oscillatory behaviour that attributes the surface wave propagation to the intermediate formation of NH species. Stable NH_2 species can be formed on Re and Fe surfaces, whereas the noble metal surfaces can form weakly stable NH_2 particles at the very edge of their existence region. The combination reaction between two NH_2 species is endothermic in all cases.

CONJUGATE ELECTRON EXCITATION IN A SUBSTRATE–ADSORBATE SYSTEM

A.R. Cholach, V.M. Tapilin

Chem. Sustain. Devel., 11(1) (2003) pp. 55–62.

The electronic peculiarities of the Pt(100)–(1x1) surface effected by various adsorbates and interactions in adsorbed layer were studied by the Disappearance Potential Spectroscopy (DAPS). Two types of features were observed in DAPS spectra. The first type corresponds to an ordinary threshold excitation of platinum core electron to an available vacant state. These features are attributed to the substrate properties, and their positions are in good agreement with corresponding Local Density of States (LDOS) calculations. The second type of features evidences for a new way of primary electron energy consumption – the conjugate electron excitation, which includes the above threshold transition of the substrate core electron, accompanied by excitation of the valence electron of adsorbed species to vacuum level. Positions of the respective spectral satellites are close to corresponding ionization potentials of a given species in adsorbed layer. The obtained experimental data show altogether more than 10 satellites, providing the evidence of reliability of the conjugate electron excitation process. The present results as a whole experimentally demonstrate the substantial unity of the substrate and adsorbate electronic structures.

CLUSTER MODEL DFT STUDY OF THE INTERMEDIATES OF BENZENE TO PHENOL OXIDATION BY N_2O ON FeZSM-5 ZEOLITES

N.A. Kachurovskaya*, G.M. Zhidomirov, E.J.M. Hensen*, R.A. van Santen* (*Schuit Institute of Catalysis, Eindhoven University of Technology, Eindhoven, The Netherlands)

Catal. Lett., 86(1) (2003) pp. 25–31.

An Fe(II) ion at an α-cation exchange position of ZSM-5 zeolite (Fe/Z) was taken as a model for the active site in the nitrous oxide decomposition and in the selective oxidation of phenol with nitrous oxide. The oxygen deposited by decomposition of N_2O is commonly referred to as α-oxygen (OFe/Z). Cluster model DFT calculations show that the interaction of the OFe/Z center with benzene resulted easily in arene oxide formation. The results indicate a rather low activation energy for this step. Possible transformations of the adsorbed arene oxide are considered and the experimental evidence for the absence of the kinetic H/D isotope effect in phenol formation is discussed. It is concluded that the rate-limiting step for the *in situ* oxidation of benzene to phenol is the desorption of the product.

MECHANISM OF DIRECT OXIDATION OF CYCLOHEXENE TO CYCLOHEXANONE WITH NITROUS OXIDE. THEORETICAL ANALYSIS BY DFT METHOD

V.I. Avdeev, S.Ph. Ruzankin, G.M. Zhidomirov

Chem. Commun., 1 (2003) pp. 42–43.

New very effective results on the liquid-phase oxidation of cyclohexene to cyclohexanone by nitrous oxide are analyzed using the B3LYP/6-31G* approximation. The calculations predict a two-step mechanism of the reaction. Actually, the reaction of cycloaddition of 1,3-dipolar to cyclohexene with nitrous oxide is the first step. The second step involves the subsequent decomposition of intermediate, formation of the target product, cyclohexanone, due to transition of hydrogen within the carbon cycle:

$$OC1H1\text{-}C2H \rightarrow O = C1\text{-}C2H_2.$$

The first step of the reaction can be considered as activation of a nitrous oxide molecule, providing the N_2O decomposition and creation of active oxygen through formation of an adduct with cyclohexene. The second step governs the nature of the desired product. It has been considered only two probable products, cyclohexanone and cyclohexene oxide. At catalytic liquid-phase oxidation of alkenes with N_2O, the reaction channel with formation of epoxides is possible. In the case of non-catalytic oxidation, this channel is eliminated.

ONEFOLD COORDINATED OXYGEN ATOM: AN ELECTRON TRAP IN THE SILICON OXIDE

V.A. Gritsenko*, A.V. Shaposhnikov*, Yu.N. Novikov*, A.P. Baraban, Hei Wong***, G.M. Zhidomirov, M. Roger****** (*Institute of Semiconductor Physics, Novosibirsk, Russia; **St. Petersburg State University, St. Petersburg, Russia; ***Department of Electronic Engineering, Kowloon, Hong Kong; ****DRECAM, SPEC, Gif sur Yvette Cedex, France)

Microelectron. Reliability, 43(4) (2003) pp. 665–669.

It has been long suggested that the SiOH defect is an electron or "water" trap in silicon dioxide based on some indirect evidences. In this work, quantum calculation on the capturing properties of non-bridging oxygen hole center with unpaired electron $SiO^{\cdot}$ and hydrogen defect SiOH in silicon oxide are performed with the *ab initio* Density-Functional Method. It was found that the $SiO^{\cdot}$ defect is an electron trap and this defect should be the responsible candidate for better hardness against radiation for the metal–oxide-semiconductor gate oxide produced by wet oxidation. It was found that the SiOH defect could not be an electron trap according to the present calculation results.

VALENCE BAND OFFSET AT SILICON/SILICON NITRIDE AND SILICON NITRIDE/SILICON OXIDE INTERFACES

V.A. Gritsenko*, A.V. Shaposhnikov*, Yu.N. Novikov*, W.M. Kwok, Hei Wong***, G.M. Zhidomirov** (*Institute of Semiconductor Physics, Novosibirsk, Russia; **Department of Chemistry, The Chinese University of Hong Kong, Shatin, Hong Kong, PR China; ***Department of Electronic Engineering, Kowloon, Hong Kong, PR China)

Thin Solid Films, 437(1-2) (2003) pp. 135–139.

The valence band electronic structure of silicon nitride (Si_3N_4) is studied using the first principal quantum chemical calculation, X-Ray photoelectron spectroscopy

(XPS) and ultraviolet photoelectron spectroscopy (UPS). Assuming that the valence band is formed with N 2p and Si 3s, 3p and 3d electrons and based on the XPS and UPS results, the valance band offset at the Si/Si_3N_4 interface was estimated to be 1.5±0.2 eV. This hole barrier explains the hole dominating conduction in Si/Si_3N_4 structure when a positive potential is applied to the silicon substrate. In addition, the UPS study reveals that the valence band offset at the Si_3N_4/silicon oxide interface is 2.5±0.2 eV.

CAPTURING PROPERTIES OF THREE-FOLD COORDINATED SILICON ATOM IN SILICON NITRIDE: POSITIVE CORRELATION ENERGY MODEL

V.A. Gritsenko*, Yu.N. Novikov*,
A.V. Shaposhnikov*, Hei Wong,**
G.M. Zhidomirov (*Institute of Semiconductor Physics, Novosibirsk, Russia; **Department of Electronic Engineering, Kowloon, Hong Kong, PR China)

Phys. Solid State,
45(11) (2003) pp. 2031-2035.

The electronic structure and capturing properties of three-fold coordinated silicon atoms ($\equiv$ Si·) and the Si–Si bond in silicon nitride (Si_3N_4) were studied using the *ab initio* Density Functional Theory. The results show that the previously proposed negative correlation energy (NCE) model is not applicable to Si_3N_4. The NCE model was proposed for interpreting the absence of the ESR signal for three-fold coordinated silicon defects and suggested that an electron can transfer between two silicon defects. It was proposed that the absence of this ESR signal is due to the creation of neutral diamagnetic Si–Si defects in Si_3N_4. This model offers the most fundamental theory for explaining the hole localization (memory) effect in silicon nitride.

ELECTRONIC STRUCTURE AND OPTICAL PROPERTIES OF SURFACE F-CENTERS OF MgO OXIDE. THE THEORETICAL ANALYSIS BY DFT METHOD

V.I. Avdeev, G.M. Zhidomirov

J. Struct. Chem., 44(6) (2003) pp. 995-1004.

Electron structures of clusters Mg_9O_9 and Mg_9O_8 that model nanocrystalline magnesia powders were analyzed in terms of the density functional theory (DFT). The surface and bulk properties of the nanocrystals were compared by time-dependent DFT (TD-DFT) analysis of variations in the density of electron states (DOS) and changes in the electron spectra. Spectroscopy of special defects, such as low-coordinated oxygen ions, and point defects, such as F^+ and F-centers, was studied. The optical properties of nanosize magnesia were shown to be characterized by a set of absorption bands at the region between 1.2 and 1.5 eV. Spatial defects O_{LC} in the nanocrystals generate absorption bands at 2.5–5.0 eV. The calculations demonstrated that there is no direct relation between the coordination number of surface ions and energy of the excited states. Theoretical energies of the excited states were compared to experimental optical properties of F^+ and F-centers.

MODELING ACTIVE CENTERS IN AMMONIA SYNTHESIS. DFT STUDY OF DISSOCIATIVE ADSORPTION OF N_2 ON Ru CLUSTERS

S.F. Ruzankin, V.I. Avdeev, N.M. Dobrynkin,
G.M. Zhidomirov, A.S. Noskov

J. Struct. Chem., 44(3) (2003) pp. 341–350.

Models of possible active centers (AC) of nitrogen adsorption on ruthenium clusters are suggested. An AC is represented by a labile Ru_n ($n = 6, 7$) cluster stabilized in carbon nanotubes. Nanotubes are modeled by the C_{60} cluster. Density Functional Theory is used to calculate the stationary points of the reaction path of dissociative adsorption of N_2 on the suggested AC. Optimal structures and transition state (TS) energies are determined. The effect of alkali metal (Cs) additions on the activation energy is investigated.

MOLECULAR MECHANISM OF ETHYLENE EPOXIDATION ON SILVER: STATE OF THE PROBLEM AND THEORETICAL APPROACHES

G.M. Zhidomirov, V.I. Avdeev, A.I. Boronin

Computer Material Science,
NATO Science Series III:
Computer and Systems Science,
V. 187 (2003) pp. 334–355.

A new concept of the oxygen species epoxidizing ethylene on silver is presented. The epoxidizing oxygen is formed on the defects of the partially oxidized metal silver surface. Oxygen saturates the bulk of silver at high temperature ($T > 500$ K) and pressure of the reaction medium, and the whole subsurface layer becomes highly defective. A cluster model of the defect structure surface AS_V, including a silver atom vacancy and the subsurface oxygen atoms is considered.

Calculations were performed in the framework of DFT approach. It was shown that the subsurface oxygen atoms tend towards self-association and formation of quasi-molecular oxygen structures inside of the vacancy space. Adsorption of the oxygen atom on site AS_V also provides stabilization of the surface quasi-molecular ("ozonide") form, $AS_V + O \rightarrow AS_d\text{-}O$.

The experimental XPS, UPS, IR, and Raman spectroscopy providing evidence in favor of stabilization of the quasi-molecular oxygen forms on the reactive silver surface are discussed. A theoretical interpretation of the experimental data is based on the proposed model of associative oxygen forms.

CO ADSORPTION ON Pd NANOPARTICLES: DENSITY FUNCTIONAL AND VIBRATIONAL SPECTROSCOPY STUDIES

I.V. Yudanov, R. Sahnoun*, K.M. Neyman*, N. Rösch*, J. Hoffmann, S. Schauermann**, V. Johanek**, H. Unterhalt**, G. Rupprechter**, J. Libuda**, H.-J. Freund**** (*Institut für Physikalische und Theoretische Chemie, Technische Universität München, Garching, Germany; **Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany)

J. Phys. Chem. B, 107(1) (2003) pp. 255–264.

Adsorption of CO on nanosize Pd particles was studied theoretically by Density Functional Method and spectroscopically by means of infrared reflection absorption spectroscopy (IRAS) and sum frequency generation (SFG).

A density functional approach was applied to three-dimensional crystallites of about 140 atoms. The model clusters were chosen as octahedral fragments of the face centered cubic (fcc) bulk, exhibiting (111) and (001) facets. Bare and adsorbate decorated cluster models were calculated with O_h symmetry constraints. Various types of adsorption sites were inspected: three-fold hollow, bridge, and on-top positions at (111) facets; four-fold hollow and on-top sites at (001) facets; bridge positions at cluster edges; on-top positions at cluster corners and on single Pd atoms deposited at regular (111) facets. Adsorption properties of the relatively small regular cluster facets (111) and (001) are calculated similar to those of corresponding ideal (infinite) Pd surfaces. However, the strongest CO bonding was calculated for the bridge positions at cluster edges. The energy of adsorption on-top of low-coordinated Pd centers (kinks) is also larger than that for on-top sites of (111) and (001) facets.

To correlate the theoretical results with spectroscopic data, vibrational spectra of CO adsorbed on supported Pd nanocrystallites of different size and structure (well-faceted and defect-rich) were measured using IRAS and SFG. For CO adsorption under ultrahigh vacuum conditions, a characteristic absorption in the frequency region 1950–1970 cm^{-1} was observed, which in agreement with the theoretical data was assigned to vibrations of bridge-bonded CO at particles edges and defects. SFG studies carried out at CO pressures up to 200 mbar showed that the edge-related species was still present under catalytic reaction conditions. By decomposition of methanol leading to the formation of carbon species, these sites can be selectively modified. As a result, CO occupies on-top positions at particle edges and defects. Based on the computational data, the experimentally observed differences in CO adsorption on alumina-supported Pd nanoparticles of different size and surface quality are interpreted. Differences between adsorption properties of Pd nanoparticles with a large fraction of (111) facets and adsorption properties of an ideal Pd(111) surface are also discussed.

A TECHNIQUE FOR CALCULATING THE ELECTRONIC STRUCTURE OF SLABS WITH ANY NUMBER OF LAYERS

V.M. Tapilin

Phys. Low-Dimens. Struct., 9/10 (2002) pp. 23–34.

A set of equations whose order is independent on a number of layers in a slab is derived for calculating the electronic structure of the slab. The sets for slab fragments of "cubium" crystal were solved for illustration. The dependence of the position of levels corresponding to the band bottom, middle of the band, a surface state, and Fermi energy and the charge distribution on a number of layers in the slab are presented. The results are identical with those obtained using the conventional technique, but the computer time needed for calculating, e.g., a 50-layer slab is 5 orders of magnitude shorter for the new technique, compared with that for the conventional procedure. The proposed technique seems to be promising in application to nanostructural materials.

NUMERICALLY INTEGRABLE CONFINED BASIS FUNCTIONS FOR BAND STRUCTURE CALCULATIONS

V.M. Tapilin

J. Struct. Chem., 44(6) (2003) pp. 987-994.

Numerical atomic and Slater functions are matched a polynomial which becomes zero at a certain preset radius. Beyond the radius, the functions are identically equal to zero. These functions with different in number continuous derivatives at matching and cutoff radii are used for band structure calculations of copper crystal. It is found that the use of Gauss quadratures not corrected for discontinuity of basis function derivatives provides the numerical integration accuracy, which is necessary for calculation of matrix elements, if the basis functions have three continuous low-order derivatives at the cutoff radius and more than four at matching radius. When the matching radius size is widely varied, the quality of the basis set is practically independent of this value. An increase in the cutoff radius improves the basis quality, the basis limit of spatially unbounded basis functions being already reached at cutoff radii shorter than double distance between the nearest neighbors. As a result, the basis set of confined functions is obtained which is not inferior to the ordinary basis of atomic or Slater functions and requires no special methods of numerical integration. At the same time, the proposed set allows the calculation time to be two times shortened.

QUANTUM-CHEMICAL CALCULATION OF MATRIX ELEMENTS IN A BASIS OF FUNCTIONS WITH POLYNOMIAL TAILS

V.M. Tapilin

J. Struct. Chem., 44(4) (2003) pp. 531–537.

A numerical integration method is suggested for calculating Hamiltonian matrix elements in a basis of functions with polynomial tails with allowance for discontinuities of higher-order derivatives of the basis function within the domain of integration. The method is tested by calculating matrix elements for a copper crystal. The results for the overlap matrix elements are presented demonstrating efficiency of the method.

GROUP-THEORETICAL ANALYSIS OF THE ELECTRONIC STRUCTURE DATA FOR MOLECULAR IONS $\mathrm{C}_{60}^{\mathrm{N}\pm}$ $(\mathrm{I_h})$ DERIVED FROM MULTIPOLE EXPANSION OF THE COULOMB INTERELECTRONIC INTERACTIONS

B.N. Plakhutin

J. Chem. Phys., 119(21) (2003) pp. 11429–11436.

The paper presents a group-theoretical analysis of the new approach to calculating molecular ions $\mathrm{C}_{60}^{\mathrm{N}\pm}$ $(\mathrm{I_h})$ based on the multipole expansion of interelectronic interactions and of the results of calculations presented by Nikolaev and Michel (N&M) in [J. Chem. Phys., 117, 4761 (2002)]. By combining the N&M method with the theory of “integral invariants” developed by Plakhutin and Judd & Lo, the basic formulae and quantities of the former method are represent in the symmetry-reduced form corresponding to a full separation of variables. This enables to derive two general relationships between multipole expansion data for complementary configurations, electronic γ^{N} and hole $(\gamma^{+})^{\mathrm{N}}$. These relationships are used to correct the numerical data (coefficients of the multipole expansion and the energies of the states) presented by N&M for the hole configurations $(t_{1u}^{+})^{\mathrm{N}}$ and $(h_{u}^{+})^{\mathrm{N}}$. Some new possible applications of the modified (symmetry-reduced) N&M method are discussed.

IR-SPECTRA OF PARACETAMOLI AND PHENACETINUM. 1. THEORETICAL CALCULATIONS AND EXPERIMENTAL STUDYING

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J. Struct. Chem., 45(1) (2004) pp. 67-76.

IR spectra were acquired for crystalline powders of paracetamol and phenacetin and their solutions in chloroform and dimethylsulfoxide. To interpret the IR spectra, ab-initio calculations of equilibrium geometry and vibrational spectra of paracetamol and phenacetin molecules were performed. Comparative data on the optimized molecule parameters and experimental bond lengths and valence angels determined for the crystalline forms of paracetamol and phenacetin allowed changes in their structure transition from isolated molecular states to crystalline state (molecular crystal) to be estimated. The differences between experimental IR spectra of solutions and crystalline samples were analyzed. The role of hydrogen bonds in structure of molecular crystals was investigated and the spectra regions that characterize maximal molecular interaction were identified.

MODELLING THE PROCESS OF WATER PENETRATION INTO SOFTWOOD CHIPS

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J. Pulp Paper Sci., 29(4) (2003) pp. 137–143.

A mathematical model was developed for the process of water penetration into softwood chips under isothermal conditions. The model takes into account several important phenomena, including capillary rise, air dissolution and outward diffusion, and the decrease in the permeability coefficient of wood as a function of the chip saturation degree. Based on this model, a computer simulation program was written to obtain quantitative information about the penetration of water into different chips under various process conditions. The program was found to predict accurately the course and final level of water penetration into the chips under defined conditions.

Monte-Carlo Simulation to Study Physico-Chemical Processes

APPLICATION OF STATISTICAL LATTICE MODELS TO THE ANALYSIS OF OSCILLATORY AND AUTOWAVE PROCESSES IN THE REACTION OF CARBON MONOXIDE OXIDATION OVER PLATINUM AND PALLADIUM SURFACES

V.I. Elokhin, E.I. Latkin, A.V. Matveev, V.V. Gorodetskii

Kinet. Catal., 44(5) (2003) pp. 692–700.

Statistical lattice models which imitate oscillatory and wave dynamics in the adsorbed layer during carbon monoxide oxidation over Pt(100) and Pd(110) single crystals differing in the mechanism of autooscillation formation are compared. In the case of platinum, oscillations are due to phase transitions of the catalyst surface structure and surface reconstruction under the action of the reaction medium. In the case of palladium, the driving force of oscillations is phase transitions in the adsorbed layers on the catalyst surface, namely, the reversible formation of subsurface oxygen in the course of the reaction, which modifies the adsorption and catalytic properties of the surface. It is shown that, according to the proposed models, a change in the coverages ($CO_{ads} \leftrightarrow O_{ads}$) in the autooscillation regimes occurs via the formation of a surface wave whose front is characterized by the high concentration of catalytically active sites that provide the maximal rate of CO_2 molecule formation. Under certain conditions, the formation of various spatiotemporal structures is observed in simulation experiments.

MANIFESTATION OF THE ADSORBED CO DIFFUSION ANISOTROPY CAUSED BY THE STRUCTURE PROPERTIES OF THE Pd(110) – (1×2) SURFACE ON THE OSCILLATORY BEHAVIOUR DURING CO OXIDATION REACTION – MONTE-CARLO MODEL

A.V. Matveev, E.I. Latkin, V.I. Elokhin, V.V. Gorodetskii

Chem. Sustain. Devel., 11(1) (2003) pp. 173–180.

The modelling of self-oscillations and surface autowaves in CO oxidation reaction over Pd(110) has been carried out by means of the Monte-Carlo technique. The synchronous oscillations of the reaction rate and surface coverages are exhibited within the range of the suggested model parameters (under the conditions very close to the experimental observations). The dependencies of the simulation results on the lattice size and on the diffusion intensity have been studied. It has been established that the adsorbed CO diffusion anisotropy does not influence the oscillation kinetics but leads to the appearance of the propagating reaction fronts on the palladium surface elliptically stretched along the [110] direction in close agreement with the known experimental data.

SPIRAL CONCENTRATION WAVES IN THE MONTE CARLO MODEL OF CO OXIDATION OVER Pd(110) CAUSED BY SYNCHRONISATION VIA CO_{ads} DIFFUSION BETWEEN SEPARATE PARTS OF CATALYTIC SURFACE

E.I. Latkin, V.I. Elokhin, V.V. Gorodetskii

Chem. Eng. J., 91(2-3) (2003) pp. 123–131.

The role of adsorbed CO diffusion as a synchronisation factor between the separate oscillating surfaces in CO oxidation reaction has been examined by means of Monte Carlo model. As a result of the chosen simulation strategy the spiral waves of adsorbed species on the palladium surface (imagined as a set of independent Pd(110) planes) have been observed. The dependence of the results on the details of the simulation experiment as well as on the size of the lattice representing the catalytic surface has been studied.

NOVEL STATISTICAL LATTICE MODEL FOR THE SUPPORTED NANOPARTICLE. FEATURES OF THE REACTION PERFORMANCE INFLUENCED BY THE DYNAMICALLY CHANGED SHAPE AND SURFACE MORPHOLOGY OF THE SUPPORTED ACTIVE PARTICLE

E.V. Kovalyov, E.D. Resnyanskii, V.I. Elokhin, B.S. Bal'zhinimaev

Phys. Chem. Chem. Phys.,
5(4) (2003) pp. 784–790.

The aim of this study is to reveal the mutual influence of the shape and the surface morphology of supported nanoparticles on the reaction kinetics. The analysis has been provided by means of the novel statistical lattice model, which imitates the physicochemical processes that proceed over the supported particles. To simulate the active metal particle the finite Kossel crystal located on the inert support has been chosen. The surface morphology of the particle is defined by distribution of heights of the metal atom columns. The metal atoms attract the nearest neighbour metal atoms and the atoms of the support. The attraction is characterised by interaction energies between the nearest neighbour metal atoms and between the metal atom and the support underneath. The change of morphology is caused by the thermal diffusion of the surface atoms. As a result the equilibrium shape of the particle has been observed to depend on the temperature and the relative ratio of metal-metal and metal-support energies. The model reaction $2A + B_2 \rightarrow 2AB$ has been studied, taking into account the roughening of the particle surface and the spillover phenomenon of the adsorbed A_{ads} over the support. It has been shown that the kinetics of the roughened nanometer-sized particle can be notably different from those corresponding to the flat homogeneous surface. The shape of the nanoparticle can change under the influence of the adsorbed layer even in the absence of the adsorbate-metal interactions.

SIMULATION OF MORPHOGENESIS: FROM A PLURIPOTENT STEM CELL TO AN ENSEMBLE OF DIFFERENTIATED CELLS

V.P. Zhdanov, B. Kasemo* (*Department of Applied Physics, Chalmers University of Technology, Goteborg, Sweden)

Phys. Chem. Chem. Phys.,
5(7) (2003) pp. 1433–1439.

Two general models are proposed describing growth of a cell population. The first mean-field model, taking into account self-driven proliferation and long-range inhibitory interactions, makes it possible to generate various types of temporal kinetics of division of differentiated cells even if cells form a simple spherical 3D structure. Asymptotically, it reproduces exponential growth, power-law growth, and termination of the growth. The second model, based on the lattice Monte Carlo technique, illustrates the role of spatial constraints and cell-cell adhesion and communication in morphogenesis occurring *via* diffusion and division of pluripotent stem cells and differentiated cells. The latter model may predict complex patterns even in the case of a relatively small number of cell types and simple rules of communication.

SIMULATION OF THE FIRST STAGE OF OXIDE FORMATION ON Al(111)

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Surf. Sci., 521(1-2) (2002) L662–L668.

At room temperature, the oxide formation on Al(111) starts on the boundaries of relatively large islands containing about or more than 20 chemisorbed oxygen atoms. It has been shown that this special feature can be rationalized by assuming that the jump rate of oxygen atoms to the subsurface layer depends on lateral oxygen–oxygen interactions in the ground and activated states. In both cases, the lateral interaction is considered to consist of two components, including attractive nearest-neighbour interaction and repulsive elastic interaction at longer distances. To explain the experimentally observed details of oxide nucleation, the attractive interaction in the activated state should be slightly weaker than in the ground state.

OSCILLATIONS IN THE NO-CO REACTION ON Pt(100): NO DECOMPOSITION ON ISLAND BOUNDARIES

V.P. Zhdanov

Catal. Lett., 84(2) (2002) pp. 147–151.

The first Monte Carlo simulations of kinetic oscillations in heterogeneous catalytic reaction is presented with one of the key reaction steps occurring on the boundaries between the islands formed due to adsorbate-induced surface restructuring. Specifically, it was treated NO reduction by CO on the Pt(100) surface with NO decomposition on the interface between the "hex" and 1x1 phases. For this scenario, in agreement with experiment, the model predicts damped oscillations with correlation between broad maxima in the CO_2-formation rate and minima in the 1x1 area.

ROLE OF STEPS IN THE NO-CO REACTION ON THE (111) SURFACE OF NOBLE METALS

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Surf. Sci., 529(3) (2003) pp. 338–348.

One of the most probable scenarios of the NO–CO reaction on the (111) surface of noble metals includes reversible NO and CO adsorption, NO dissociation, N_2 desorption, and CO_2 formation due to reaction between adsorbed CO and O species. Adopting this scheme, the reaction kinetics was analyzed in the situation when the surface contains steps. Employing the mean-field kinetic equations with the kinetic parameters corresponding to the case when the adsorbate coverage is high and the reaction rate is limited by NO dissociation, it has been shown that the contribution of steps to the reaction rate may be appreciable. The adsorbate–diffusion-mediated communication between terraces and steps can play a constructive role in the reaction, i.e., the reaction rate may be higher with than without communication. In addition, Monte Carlo simulations is presented demonstrating that, due to limitations in the rate of N diffusion, the adsorbate distribution along the surface may be non-uniform with the largest N coverage near steps. Such reaction regimes are found to be possible even for relatively high rates of N diffusion (e.g., in the case when the ratio of the rates of N jumps and CO or NO impingement is about 10^4). The implications of these findings for the understanding of the specifics of the reaction under consideration are briefly discussed.

ONE OF THE SCENARIOS OF ELECTROCHEMICAL OXIDATION OF CO ON SINGLE-CRYSTAL Pt SURFACES

V.P. Zhdanov, B. Kasemo* (*Department of Applied Physics, Chalmers University of Technology, Göteborg, Sweden)

Surf. Sci., 545(1–2) (2003) pp. 109–121.

Monte Carlo simulations is presented illustrating that the transient potential-step kinetics of CO oxidation on single-crystal Pt surfaces are fairly sensitive to adsorbate–adsorbate lateral interactions. Specifically, it has been shown that with realistic values of these interactions ≅1 kcal/mol) the reaction kinetics may be accompanied by CO segregation provided that surface CO diffusion is fast. In addition, it was demonstrated that the CO-island formation might be one of the reasons of extinction in CO oxidation. Implications of these findings for interpretation of experimental data are discussed.

ROLE OF THE FIELD FLUCTUATIONS IN ELECTROCHEMICAL REACTIONS

V.P. Zhdanov, B. Kasemo* (*Department of Applied Physics, Chalmers University of Technology, Goteborg, Sweden)

Appl. Surf. Sci., 219(3-4) (2003) pp. 256–263.

Rate constants of electrochemical reactions, accompanying by electron transfer via the electrolyte–metal interface, exponentially depend on the electrode potential. Monte Carlo simulations is presented illustrating the effect of fluctuations of the potential near the reactants on the rate of such reactions. The two models employed are based on the phenomenological Frumkin theory and aimed, respectively, at conventional electrolytes and polymer electrolytes widely used in fuel cells. In both cases, the role of spatio-temporal fluctuations is found to be minor if the dielectric constant in the double layer is large, ≅ 80 (as in the bulk water). If the double-layer dielectric constant is smaller, e.g. ≅ 30 as it often takes place in conventional and polymer electrolytes, the fluctuations result in appreciable increase of the apparent reaction rate constant. This effect is especially important (of a factor of 15) for polymer electrolytes. In the latter case, the reaction rate is actually controlled by the fluctuations. Implications of these findings for basic and applied electrochemistry are briefly discussed.

SIMULATION OF KINETIC OSCILLATIONS IN THE CO+O_2/Pt REACTION ON THE nm SCALE

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J. Catal., 214(1) (2003) pp. 121–129.

Kinetic oscillations in CO oxidation occurring on nm-sized supported Pt particles via the conventional Langmuir-Hinshelwood mechanism and surface oxide formation and removal were simulated using the Monte Carlo technique. Incorporating cooperative effects into the oxide growth mode, it was demonstrated that the oscillations may be accompanied by remarkable segregation between oxide and CO. During oscillations, the maximum CO coverage may be appreciably smaller that that at saturation. These findings are in line with recent transient Fourier transform infrared spectroscopy measurements [Fanson, P.T., et al., J. Catal. 204, 35 (2001)] indicating that during oscillations on Pt/SiO_2 the CO coverage is relatively low and the shift of the stretching frequency of linearly bonded CO is nearly negligible.

NON-MARKOVIAN KINETICS OF RAPID LONG-RANGE INTERPROTEIN ELECTRON TRANSFER

V.P. Zhdanov

Europhys. Lett., 62(5) (2003) pp. 643–649.

Using a lattice Monte Carlo model describing electron tunneling between an electron donor, linked with a beta sheet, and an electron acceptor, it was shown how electron-induced protein reconfiguration may result in non-Markovian features in the long-range electron-transfer kinetics.

Physicochemical Methods to Study Active Sites, Mechanism and Reaction Kinetics

MULTINUCLEAR NMR STUDY OF THE REACTIVE INTERMEDIATES IN ENANTIOSELECTIVE EPOXIDATIONS OF ALLYLIC ALCOHOLS CATALYZED BY A VANADIUM COMPLEX DERIVED FROM A PLANAR-CHIRAL HYDROXAMIC ACID

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New J. Chem., 27(3) (2003) pp. 609–614.

Structure and reactivity of vanadium(V) complexes formed *in situ* in the catalytic system VO(Oalkyl)$_3$/hydroxamic acid/*tert*-butylhydroperoxide (TBHP) have been examined by means of ^{51}V, ^{13}C and ^{17}O NMR spectroscopy. For the first time, reactive vanadium(V) alkylperoxo intermediates in vanadium/hydroxamic acid epoxidations were observed and spectroscopically characterized. With a planar-chiral [2.2]paracyclophane-derived hydroxamate as ligand two diastereomeric alkylperoxo vanadium(V) complexes were formed in a 3:1 ratio. They differ in the relative positioning of the VO group and the planar-chiral aromatic part. Upon addition of geraniol as substrate, these complexes disappear in a parallel manner, and geraniol epoxide is formed. Probably, the existence of these two diastereomeric complexes and their comparable reactivity account for the observed enantioselectivity level and hence sets a fundamental limitation for the use of such ligands in this asymmetric catalysis.

STEREOSELECTIVE OXIDATION OF LINALOOL WITH *TERT*-BUTYL HYDROPEROXIDE, CATALYZED BY A VANADIUM(V) COMPLEX WITH A CHIRAL TERPENOID LIGAND

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J. Mol. Catal. A: Chem.,
194(1-2) (2003) pp. 79–88.

Stereoselective epoxidation of (−)-(*R*)-linalool by *tert*-butylhydroperoxide (TBHP) catalyzed by a vanadium(V) complex formed by interaction of [VO(acac)$_2$] or [VO(O*n*-Bu)$_3$] with a new chiral terpenoid ligand (L) is reported. Moderate diastereomeric excess (*de* 56 %) was attained in toluene at 20 °C. ^{51}V, ^{13}C and ^{17}O NMR spectroscopic monitoring of the studied catalytic system showed that a new complex **1** forms quantitatively upon interaction of [VO(O*n*-Bu)$_3$] with L in CH_2Cl_2. Compound **1** is a mononuclear complex of vanadium(V), which incorporates the tridentate chiral ligand L, as well as V = O moieties. It has been shown that TBHP binds to **1** giving a **1**·TBHP adduct with the association constant $K = 1.36\pm0.11\ l\cdot mol^{-1}$ at room temperature and enthalpy $\Delta_r H_{298}^0 = -6.5\pm2.0$ kJmol^{-1} and entropy $\Delta_r S_{298}^0 = -20\pm6$ Jmol^{-1}K^{-1}. These thermodynamic parameters are typical for outer sphere complexes (OSCs). Adduct **1**·TBHP is suggested to be a precursor of the active intermediate of the stereoselective epoxidation process.

INTERMEDIATES OF ASYMMETRIC OXIDATION PROCESSES CATALYZED BY VANADIUM(V) COMPLEXES

K.P. Bryliakov, E.P. Talsi

Kinet. Catal., 44(3) (2003) pp. 334-346.

The [VO(acac)$_2$]/Schiff base [*R*-2-(*N*-3,5-di-*tert*-butylsalicylidene)amino-2-phenyl-1-ethanol, *S*-2-(*N*-3,5-di-*tert*-butylsalicylidene)amino-3,3-dimethyl-1-butanol, *S*-2-(*N*-3,5-di-*tert*-butylsalicylidene)amino-3-methyl-1-butanol, or *R*-2-(*N*-3,5-di-*tert*-butylsalicylidene) amino-3-phenyl-1-propanol]/H_2O_2 catalytic systems for the asymmetric oxidation of sulfides and the [VO(acac)2]/(3b*R*,4a*R*)-2-(3,4,4-trimethyl-3*b*,4,4*a*,5-tetrahydrocyclopropa[3,4]cyclopenta[1,2-*c*]pyrazol-1-yl) ethanol/*tert*-butylhydroperoxide/TBHP and VO(OAlkyl)$_3$/[2,2]paracyclophane-4-carboxylic acid *N*-(1,1-dimethylethyl)-*N*-hydroxamide/TBHP catalytic systems for the asymmetric epoxidation of allylic alcohols were studied using ^{13}C, ^{51}V, and ^{17}O NMR spectroscopy. The key intermediates of these systems (peroxo and alkylperoxo complexes of vanadium(V)) were detected, their structures in solution were studied, and the reactivity was evaluated.

MULTINUCLEAR NMR-SPECTROSCOPIC CHARACTERIZATION OF ALKYLPEROXO COMPLEXES OF MOLYBDENUM(VI)

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Mendeleev Commun., 13(1) (2003) pp. 8–9.

Molybdenum catalysed epoxidation with organic hydroperoxides remains the basis for the industrial production of propylene oxide, as well as a convenient laboratory method for the epoxidation of more complicated alkyl olefins. It is generally agreed that alkylperoxo molybdenum complexes are the active species of these reactions. However, up to date the alkylperoxo complexes of molybdenum have neither been isolated, nor sufficiently characterized spectroscopically. For the highly active and practically attractive molybdenum based catalytic systems, the rate of epoxidation of olefins with organic hydroperoxides was shown to be independent on the nature of the molybdenum complex used as the starting material for the catalyst, and the starting complex was converted in the course of the reaction into complexes of molybdenum(VI) with 1,2-alkane-diol (the side product of epoxidation). Thus, in order to model the practical molybdenum based epoxidising systems, it is important to characterize the alkylperoxo complexes formed in the reaction of organic hydroperoxide with 1,2-alkane-diolo molybdenum(VI) species. In this work, the alkylperoxo molybdenum(VI) intermediate formed in the reaction of ^{t}BuOOH with 1,2-cyclohexane-diolo complex of molybdenum(VI) in $CHCl_3$ was characterized for the first time by means of ^{13}C, ^{17}O and ^{95}Mo NMR spectroscopy. This intermediate is the active species of molybdenum catalysed epoxidation of cyclohexene with ^{t}BuOOH.

STABILITY OF LOW-SPIN FERRIC HYDROPEROXO AND ALKYLPEROXO COMPLEXES WITH TRIS(2-PYRIDYLMETHYL)AMINE

M.V. Lobanova, K.P. Bryliakov, E.A. Duban, E.P. Talsi

Mendeleev Commun., 13(4) (2003) pp. 175–177.

Quantitative data on the stability and reactivity of the peroxidic intermediates $[Fe^{III}(TPA)(OOH)L](ClO_4)_2$ and $[Fe^{III}(TPA)(OOBu^t)L](ClO_4)_2$ [TPA = tris(2-pyridylmethyl)amine; L = MeCN, H_2O, MeOH and Py] were obtained for the first time.

^{1}H NMR CHARACTERIZATION OF INTERMEDIATES FORMED BY THE ACTIVATION OF ZIRCONOCENES WITH METHYLALUMINOXANE AT HIGH Al/Zr RATIOS

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Mendeleev Commun., 13(3) (2003) pp. 46–48.

Cation-like intermediates formed by the activation of zirconocenes L_2ZrCl_2 [L_2 are cyclopentadienyl (Cp), indenyl (Ind) and fluorenyl (Flu) ligands] with methylaluminoxane (MAO) at high Al/Zr ratios were characterized by ^{1}H NMR spectroscopy.

^{1}H-NMR SPECTROSCOPIC STUDY OF CATIONIC INTERMEDIATES IN SOLVENT AND OIL CONSTITUENTS OF THE CATALYTIC SYSTEMS $Cp_2ZrMe_2/[CPh_3][B(C_6F_5)_4]$ AND $Cp_2ZrMe_2/AlMe_3/[CPh_3][B(C_6F_5)_4]$

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J. Organomet. Chem., 677(1-2) (2003) pp. 10–14.

Using ^{1}H-NMR spectroscopy, mutual transformations and stability of cationic complexes $[(Cp_2ZrMe)_2(\mu\text{–}Me)]^+[B(C_6F_5)_4]^-$ (**1**), $[Cp_2ZrMe^+...B(C_6F_5)_4^-]$ (**2**) and `$[Cp_2Zr(\mu\text{-}Me)_2AlMe_2]^+$ Me–MAO$^-$ (**3**) formed in catalytic systems $Cp_2ZrMe_2/[CPh_3][B(C_6F_5)_4]$ and $Cp_2ZrMe_2/AlMe_3/[CPh_3][B(C_6F_5)_4]$ in benzene were studied both in the solution and in the oil deposit formed whenever the total zirconocene concentration is high enough. It was shown that at high zirconocene concentrations, the decay rate of complexes **1** and **2** in the oil constituent of the reaction mixture is at least a factor ten lower than that in the solvent. Complexes **1-3** are close in energy to each other and can be readily converted to one another by changing the ratio between Cp_2ZrMe_2, $[CPh_3][B(C_6F_5)_4]$ and $AlMe_3$. Complex **1** reacts with excess $[CPh_3][B(C_6F_5)_4]$ to yield **2** with first order rate constant of 4×10^{-4} s^{-1} at 20 °C. Complex **3** reacts with excess $[CPh_3][B(C_6F_5)_4]$ to yield 2 with half-life of 1h at 20 °C. Addition of 1-hexene to samples containing various relative amounts of complexes **1-3**, and further ^{1}H-NMR spectroscopic monitoring of the polymer/monomer ratio, showed that **1-3** have comparable polymerization activities.

^{1}H AND ^{13}C NMR STUDY OF THE INTERMEDIATES FORMED BY $(Cp\text{-}R)_2ZrCl_2$ ACTIVATION WITH MAO AND $AlMe_3/[CPh_3][B(C_6F_5)_4]$. CORRELATION OF SPECTROSCOPIC AND ETHENE POLYMERIZATION DATA

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Macromol. Chem. Phys., 204(8) (2003) pp. 1110-1117.

Using ^{1}H and ^{13}C NMR spectroscopy, cationic intermediates formed by activation of $(Cp\text{-}R)_2ZrCl_2$ (R =*n*Bu, *t*Bu and 1,2,3-Me_3) with MAO in toluene were monitored at Al/Zr ratios from 50 to 1000. The catalysts $(Cp\text{-}R)_2ZrCl_2/AlMe_3/CPh_3^+B(C_6F_5)_4^-$ (*n*Bu, *t*Bu and 1,2,3-Me_3) were also studied for comparison of spectroscopic and polymerization data with MAO based systems. Complexes of type $(Cp\text{-}R)_2ZrMe^+\leftarrow Me^-\text{-}Al\equiv MAO$ (**IV**) with different Me-MAO$^-$ counter anions have been identified in the $(Cp\text{-}R)_2ZrCl_2$/MAO systems at low Al/Zr ratios. At Al/Zr ratios of 200–1000, the complex $[(Cp\text{-}R)_2Zr(\mu\text{-}Me)_2AlMe_2]^+$ Me-MAO$^-$ (**III**) dominates in all MAO-based reaction systems. Ethene polymerization activity strongly depends on the Al/Zr ratio (Al/Zr = 200-1000) for the systems $(Cp\text{-}n\text{Bu})_2ZrCl_2$/MAO and $(Cp\text{-}t\text{Bu})_2ZrCl_2$/MAO while it is virtually constant in the same range of Al/Zr ratios for the catalytic system $(Cp\text{-}1,2,3\text{-}Me_3)_2ZrCl_2$/MAO. The data obtained are interpreted on assumption that complex **III** is actual precursor of active centers of polymerization in MAO based systems.

^{1}H, ^{13}C NMR AND ETHYLENE POLYMERIZATION STUDY OF ZIRCONOCENE/MAO CATALYSTS: EFFECT OF THE LIGAND STRUCTURE ON THE FORMATION OF ACTIVE INTERMEDIATES AND POLYMERIZATION KINETICS

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J. Organomet. Chem., 683(1) (2003) pp. 92–102.

Using ^{1}H- and ^{13}C-NMR spectroscopies, cationic intermediates formed by activation of L_2ZrCl_2 with methylaluminoxane (MAO) in toluene were monitored at Al/Zr ratios from 50 to 1000 (L_2 are various cyclopentadienyl (Cp), indenyl (Ind) and fluorenyl (Flu) ligands). The following catalysts were studied: $(Cp\text{-}R)_2ZrCl_2$ (R=Me, 1,2-Me_2, 1,2,3-Me_3, 1,2,4-Me_3, Me_4, Me_5, *n*-Bu, *t*-Bu), rac-ethanediyl$(Ind)_2ZrCl_2$, rac-$Me_2Si(Ind)_2ZrCl_2$, rac-Me_2Si(1-Ind-2-Me)$_2ZrCl_2$, rac-ethanediyl(1-Ind-4,5,6,7-H_4)$_2ZrCl_2$, (Ind-2-Me)$_2ZrCl_2$, $Me_2C(Cp)(Flu)ZrCl_2$, Me_2C(Cp-3-Me)(Flu)$ZrCl_2$ and $Me_2Si(Flu)_2ZrCl_2$. Correlations between spectroscopic and ethene polymerization data for catalysts $(Cp\text{-}R)_2ZrCl_2$/MAO (R=H, Me, 1,2-Me_2, 1,2,3-Me_3, 1,2,4-Me_3, Me_4, Me_5, *n*-Bu, *t*-Bu) and rac-$Me_2Si(Ind)_2ZrCl_2$ were established. The catalysts $(Cp\text{-}R)_2ZrCl_2/AlMe_3/CPh_3^+B(C_6F_5)_4^-$ (R=Me, 1,2-Me_2, 1,2,3-Me_3, 1,2,4-Me_3, Me_4, *n*-Bu, *t*-Bu) were also studied for comparison of spectroscopic and polymerization data with MAO-based systems. Complexes of type $(Cp\text{-}R)_2ZrMe^+ \leftarrow Me^-\text{-}Al{\equiv}MAO$ (**IV**) with different $[Me\text{-}MAO]^-$ counteranions have been identified in the $(Cp\text{-}R)_2ZrCl_2$/MAO (R=*n*-Bu, *t*-Bu) systems at low Al/Zr ratios (50–200). At Al/Zr ratios of 500–1000, the complex $[L_2Zr(\mu\text{-}Me)_2AlMe_2]^+[Me\text{-}MAO]^-$ (**III**) dominates in all MAO-based reaction systems studied. Ethene polymerization activity strongly depends on the Al/Zr ratio (Al/Zr=200–1000) for the systems $(Cp\text{-}R)_2ZrCl_2$/MAO (R=H, Me, *n*-Bu, *t*-Bu), while it is virtually constant in the same range of Al/Zr ratios for the catalytic systems $(Cp\text{-}R)_2ZrCl_2$/MAO (R=1,2-Me_2, 1,2,3-Me_3, 1,2,4-Me_3, Me_4) and rac-$Me_2Si(Ind)_2ZrCl_2$/MAO. The data obtained are interpreted on assumption that complex **III** is the main precursor of the active centers of polymerization in MAO-based systems.

^{13}C AND ^{1}H NMR STUDY OF Ti(IV) SPECIES FORMED BY Cp^*TiMe_3 AND Cp^*TiCl_3 ACTIVATION WITH METHYLALUMINOXANE (MAO)

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Using ^{13}C- and ^{1}H-NMR spectroscopy, titanium(IV) species formed in the catalytic systems Cp^*TiMe_3/MAO and Cp^*TiCl_3/MAO ($Cp^*=C_5(CH_3)_5$) in toluene and chlorobenzene were studied within the temperature range 253–293 K and at Al/Ti ratios 30–300. It was shown that upon activation of Cp^*TiMe_3 with methylaluminoxane (MAO) mainly the `cation-like' intermediate $Cp^*Me_2Ti^+ \leftarrow Me^-\text{---}Al(MAO)$ (**2**) is formed. Three types of titanium(IV) complexes were identified in $Cp^*TiCl_3$/MAO catalytic system. They are methylated complexes $Cp^*TiMeCl_2$ and $Cp^*TiMe_2Cl$, and the `cation-like' intermediate **2**. Complex **2** dominates in Cp^*TiCl_3/MAO system in conditions approaching to those of practical polymerization (Al/Ti ratios more than 200). According to the EPR measurements, the portion of EPR active Ti(III) species in the Cp^*TiCl_3/MAO system is smaller than 1% at Al/Ti=35, and is about 10% at Al/Ti=700.

FORMATION, SOLUTION STRUCTURE AND REACTIVITY OF ALKYLPEROXO COMPLEXES OF TITANIUM

D.E. Babushkin, E.P. Talsi

J. Mol. Catal. A: Chem.,
200(1-2) (2003) pp. 165–175.

The following titanium alkylperoxo complexes were characterized *in situ*: $Ti(\eta^2\text{-}OOtBu)_n(OiPr)_{4-n}$ (n=1–4), $[(iPrO)_3Ti(\mu\text{-}OiPr)_2Ti(OiPr)_2(\eta^2\text{-}OOtBu)]$, $[(\eta^2\text{-}OOtBu)(iPrO)_2Ti(\mu\text{-}OiPr)_2Ti(OiPr)_2(\eta^2\text{-}OOtBu)]$, $Ti(LL)_2(OR)(\eta^2\text{-}OOtBu)$, $Ti(LL)_2(\eta^2\text{-}OOtBu)_2$ and $Ti(LL)_2(OtBu)(\eta^1\text{-}OOtBu)$, where R = Et, *i*Pr; HLL = acetylacetone, dipivaloylmethane.

A detailed *in situ* ^{13}C and ^{1}H NMR spectroscopic characterization of the following families of alkylperoxo complexes of titanium is presented: $Ti(\eta^2\text{-}OOtBu)_n(OiPr)_{4-n}$, where $n = 1$–4; binuclear complexes $[(iPrO)_3Ti(\mu\text{-}OiPr)_2Ti(OiPr)_2(\eta^2\text{-}OOtBu)]$ and $[(\eta^2\text{-}OOtBu)(iPrO)_2Ti(\mu\text{-}OiPr)_2Ti(OiPr)_2(\eta^2\text{-}OOtBu)]$;

complexes with β-diketonato ligands: $Ti(LL)_2(OEt)(\eta^2\text{-}OO\mathit{t}Bu)$, $Ti(LL)_2(O\mathit{i}Pr)(\eta^2\text{-}OO\mathit{t}Bu)$, $Ti(LL)_2(\eta^2\text{-}OO\mathit{t}Bu)_2$, $Ti(LL)_2(O\mathit{t}Bu)(\eta^1\text{-}OO\mathit{t}Bu)$, where HLL = acetylacetone, dipivaloylmethane. These alkylperoxo complexes could not be isolated due to their instability and were studied *in situ* at low temperatures. Whereas the side-on (η^2) coordination mode of *tert*-butylperoxo ligand is generally preferable, the end-on (η^1) coordination caused by spatial hindrance from surrounding bulky ligands is found in two cases. The quantitative data on the reactivity of alkylperoxo complexes found towards sulfides and alkenes were obtained. The system $TiO(acac)_2/\mathit{t}BuOOH$ in C_6H_6 was reinvestigated using ^{13}C and ^1H NMR spectroscopy. The structure of the complex $Ti(acac)_2\{CH_3C(O)(OO\mathit{t}Bu)COO\}$ actually formed in this system was elucidated. Four types of titanium(IV) alkylperoxo complexes were detected in the Sharpless–Katsuki catalytic system using ^{13}C NMR spectroscopy.

IN SITU ^{1}H NMR IMAGING STUDY OF PROPAGATION OF CONCENTRATION WAVES IN AN AUTOCATALYTIC REACTION IN A FIXED GRANULAR BED

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Kinet. Catal., 44(3) (2003) pp. 401–407.

The *in situ* ^{1}H NMR technique was used to study the propagation of chemical waves during the liquid-phase Belousov–Zhabotinsky (BZ) reaction in a model fixed bed of grains consisting of chemically inert glass beads or quartz sand. The propagation of autocatalytic chemical waves in this bed is determined by the size of pores between the grains. The rate of wave front propagation is independent of the size of the grains involved in this bed but is much lower than that in the bulk of the homogenous aqueous phase. This may be attributed to the difference in the effective diffusion coefficients in the homogeneous liquid phase and in the bed.

INVESTIGATION OF HETEROGENEOUS CATALYTIC REACTIONS BY THE *IN SITU* ^{1}H NMR MICROIMAGING

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Chem. Sustain. Devel.,
11(1) (2003) pp. 109–116.

The NMR microimaging is used for the first time as an *in situ* method to study two model three-phase heterogeneous catalytic reactions with strong exothermicity. It is shown for the α-methylstyrene hydrogenation that in the course of the reaction, two domains coexist inside the catalyst grain which differ in the liquid phase content. The 2*D* maps of the liquid distribution in the course of this reaction are obtained. The reaction of the hydrogen peroxide decomposition at moderate activity of the catalyst and the H_2O_2 concentrations in the range of (0.03–3) M is shown to occur only in a thin layer near the catalyst surface. The influence of the medium inhomogeneity on the behaviour of the Belousov – Zhabotinsky chemical oscillator reaction is investigated as well.

HYDROGEN PEROXIDE DECOMPOSITION IN AQUEOUS ALKALI SUSPENSIONS OF Fe(III) OXIDE: THE NATURE OF THE ACTIVE COMPONENT

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Kinet. Catal., 44(1) (2003) pp. 86–90.

The nature of the catalytically active components is studied in the steady-state decomposition of hydrogen peroxide in alkali media in the presence of a Fe_2O_3 suspension at 25 °C in an intensively shaken reactor. It was found that a hydroxide colloid formed by the mechanical abrasion of the solid catalyst in an aqueous solution shows noticeable catalytic activity together with the initial solid-phase catalyst. As a result, the rate of the catalytic reaction becomes nonlinear with respect to the overall catalyst concentration.

REACTIVITY OF THE PEROXO COMPLEXES OF COPPER(II) HYDROXIDE

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Kinet. Catal., 44(2) (2003) pp. 211–220.

In the interaction with H_2O_2 in an alkaline medium, $Cu(OH)_2$ forms terminal Cu–OOH and bridging peroxo complexes with the μ-1,1 and μ-η^2:η^2 structures. It was found that the terminal peroxide is active in the reactions of H_2O_2 decomposition, diphenol oxidation, and nitrile conversion into acid amides. The promoting effect of ammonia on these reactions was found. A possible mechanism is discussed.

THEORETICAL AND EXPERIMENTAL STUDIES OF THE NATURE OF THE CATALYTIC ACTIVITY OF VO_X/TiO_2 SYSTEMS

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Kinet. Catal., 44(5) (2003) pp. 710–717.

The states of supported vanadium and the nature of activation of ammonia adsorbed on vanadium sites of VO_x/TiO_2 catalysts are studied by ^{51}V NMR spectroscopy and diffuse-reflectance IR Fourier-transform (DRIFT) spectroscopy using cluster quantum chemical calculations of NH_3 adsorption. The VO_x/TiO_2 catalyst of two types were employed: the monolayer catalyst in which vanadium is located on the surface of well-crystallized anatase and the catalyst in which vanadium embedded in the anatase lattice at a rather great depth. It is shown that ammonia is predominantly adsorbed on Lewis acid sites of the monolayer catalyst, whereas most of NH_3 adsorbed on the catalyst containing bulk vanadium is in the form of ammonium ions. Analysis of experimental and calculated data suggests that, in the monolayer catalyst, NH_3 molecules in the selective reduction of nitrogen oxides are activated on Lewis acid sites. Ammonia activation involves the dissociation of the N–H bond in a coordinated molecule, which results in the formation of the amide V-NH_2 group and a water molecule coordinated by a V^{5+} ion. It is likely that, in the case of the catalyst containing bulk vanadium, this reaction occurs with the predominant participation of ammonium ions.

N-BUTANE CONVERSION ON SULFATED ZIRCONIA: THE MECHANISM OF ISOMERIZATION AND ^{13}C-LABEL SCRAMBLING AS STUDIED BY *IN SITU* ^{13}C MAS NMR AND *EX SITU* GC-MS

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J. Catal., 220(1) (2003) pp. 233–239.

Using ^{13}C MAS NMR, conversion of selectively ^{13}C-labeled *n*-butane on sulfated zirconia catalyst has been demonstrated to proceed initially via two parallel routes: scrambling of the selective ^{13}C label in the *n*-butane molecule and selective formation of isobutane. The combination of the results obtained by both *in situ* ^{13}C MAS NMR and *ex situ* GC-MS analysis provides evidence for the monomolecular mechanism of the ^{13}C-label scrambling, whereas isomerization into isobutane proceeds through a pure bimolecular mechanism. Further, the intermolecular mechanism of *n*-butane isomerization is complicated and turns into conjunct polymerization. Besides isobutane, conjunct polymerization gives also the products of butane disproportionation, propane and pentanes, as well as the stable cyclopentenyl cations; the latter may be in charge of catalyst deactivation.

THE STUDY OF THE NATURE OF ADSORBED SPECIES TO BUILD A BRIDGE BETWEEN SURFACE SCIENCE AND CATALYSIS: PROBLEMS OF PRESSURE AND MATERIAL GAP

V.I. Bukhtiyarov

Kinet. Catal., 44(3) (2003) pp. 420–431.

This review substantiates the molecular approach to the study of the catalytic action of various systems, which consists in the comparative study of the nature and reactivity of adsorbed species and considering the problems of pressure and material gaps. The pressure gap problem can be solved by a continuous increase in the pressure of the reaction mixture, including carrying out *in situ* studies. The solution to the problem of material gap is possible when one passes from bulk to dispersed samples, which model real supported catalysts. As the last step that can build a bridge between surface science and catalysis, the study of nanoparticle reactivity toward the reactants of a catalytic reaction with varying sizes of nanoparticles is proposed. The scope of such an approach is demonstrated by the study of silver catalysts of ethylene epoxidation. It was found that the catalytic action of silver in the process of ethylene oxide synthesis is determined by the possibility of formation of electrophilic adsorbed atomic oxygen. Its formation is more efficient under the action of reaction mixtures at high pressures and on the surfaces of silver species with sizes smaller than 50 nm. It is shown that the reaction center should also contain the nucleophilic form of O_{ads}, which itself is only active in the complete oxidation of ethylene but creates the Ag^{1+} sites for ethylene adsorption. The disappearance of O_{nucl} with a decrease in the size of silver particles below 50 nm leads to a drastic decrease in the rate of ethylene epoxidation. The reaction mechanism made it possible to propose systems with an abnormally high value of selectivity to ethylene oxide (>90%).

ATOMIC OXYGEN SPECIES ON SILVER: PHOTOELECTRON SPECTROSCOPY AND X-RAY ABSORPTION STUDIES

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Phys. Rev. B: *Condens. Matter*, 67(23) (2003) 235422 (12 pages).

Two oxygen species, which are constituents of the active centers for ethylene epoxidation over silver, have been characterized by a number of physical methods sensitive to adsorbate electronic structure such as X-Ray photoelectron, ultraviolet photoelectron, Auger, and X-Ray-absorption near-edge structure spectroscopy. One of the species denoted as nucleophilic oxygen due to its activity in total oxidation only exhibits spectroscopic characteristics close to those of bulk Ag_2O. This allows to describe this species as atomically adsorbed oxygen in the structure of surface silver(I) oxide. The considerable extent of the covalency in bonding of this oxide like oxygen with the silver surface due to hybridization of O2*p* levels with Ag4*d* and Ag5*sp* orbitals should be also emphasized. Contrary to this, only 5*sp* orbitals of silver hybridize with 2*p* orbitals of oxygen as the other oxygen species forms. As a consequence, this species being also atomic oxygen is characterized by a lower oxygen-silver bonding interaction and a lower charge on the oxygen. The latter causes the activity of this electrophilic species in epoxidation. Possible models of adsorption centers for these oxygen species are discussed.

THE NATURE OF ELECTROPHILIC AND NUCLEOPHILIC OXYGEN ADSORBED ON SILVER

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Kinet. Catal., 44(3) (2003) pp. 432–440.

Results of a spectroscopic study of two forms of adsorbed atomic oxygen on a silver surface, which participate in ethylene epoxidation reaction, are presented. The possibility of the combined use of the methods of photoelectron spectroscopy and X-Ray absorption for a detailed analysis of adsorbate electron structure on solid surfaces is demonstrated. It is found that a significant difference in the position of O 1*s* lines for nucleophilic (528.3 eV) and electrophilic (530.4 eV) oxygen is determined by the effects of the initial state, that is, by the difference in the charge state of oxygen anions. The use of the well-know correlation of the Auger line splitting with a Pauling charge at an oxygen atom showed a substantial difference (~1 electron charge unit) in charge transfer from metal to the nucleophilic or electrophilic adsorbed oxygen atom. Based on the X-Ray absorption data of the oxygen *K*-edge, it is found that there is a substantial overlap of the 4*d*- and 5*sp* orbitals of silver with oxygen 2*p* orbitals in the nucleophilic state in the formation of an Ag–O bond and there is only an overlap of 5*sp* orbitals of silver with oxygen 2*p* orbitals in the electrophilic state. Structural models of the adsorption site are presented for both states. The conclusion is drawn that the charge state of oxygen in oxide systems may depend substantially on its binding to metal atoms.

IN SITU STUDY OF SELECTIVE OXIDATION OF METHANOL TO FORMALDEHYDE OVER COPPER

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React. Kinet. Catal. Lett., 79(1) (2003) pp. 181–188.

Selective methanol oxidation to formaldehyde over polycrystalline copper has been studied with the use of *in situ* XPS combined with mass spectrometry. It has been shown that the copper surface completely covered by methoxy groups exhibits low activity in methanol oxidation, whereas the metallic copper with sub-oxide oxygen is active in the selective oxidation of methanol to formaldehyde. The concentration of the sub-oxide oxygen species seems to correlate with the rate of formaldehyde production.

IN SITU STUDY OF THE SELECTIVE OXIDATION OF METHANOL TO FORMALDEHYDE ON COPPER

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Kinet. Catal., 44(5) (2003) pp. 662–668.

Combined use of X-Ray photoelectron spectroscopy (XPS) and *in situ* mass spectrometry made it possible to simultaneously obtain the O1*s* spectra and the mass spectrometric signal of formaldehyde (m/z = 30) in the course of heating (420–670 K) of polycrystalline foil in a flow of the reaction mixture of methanol and oxygen (with a total pressure of 0.1 mbar and a ratio of 3/1). It is shown that the O1*s* spectra contain two lines with E_b = 530.1 and 531.2 eV, whose relative intensities depend on the sample temperature. At a low temperature (420 K) the line with a lower binding energy dominates, whereas sample heating leads to a drastic decrease in its intensity and its replacement by a line with a higher value of E_b. A decrease in the intensity of the latter line occurs at $T > 550$ K, in the same temperature range as a drastic increase in the intensity of the formaldehyde signal. These lines were assigned on the basis of literature data and data obtained by the authors for the known forms of oxygen on copper and for the intermediate species of the reaction, such as methoxy and formate. The O1*s* line with E_b = 530.1 eV was assigned to methoxy groups, and the line with E_b = 531.2 eV was assigned to suboxide oxygen. The correlation of the intensity of the XPS signal of suboxide oxygen with the yield of formaldehyde was supported by stationary experiments using *in situ* XPS that prove its participation in the key step of the selective oxidation of methanol to formaldehyde.

COMPARATIVE XPS STUDY OF Al_2O_3 AND CeO_2 SULFATION IN REACTIONS WITH SO_2, $SO_2 + O_2$, $SO_2 + H_2O$, AND $SO_2 + O_2 + H_2O$

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Kinet. Catal., 44(4) (2003) pp. 575–582.

The interactions of Al_2O_3, CeO_2, Pt/Al_2O_3, and Pt/CeO_2 films with SO_2, $SO_2 + H_2O$, $SO_2 + O_2$, and $SO_2 + O_2 + H_2O$ in the temperature range 300–673 K at the partial pressures of SO_2, O_2, and H_2O equal to 1.5×10^2, 1.5×10^2, and 3×10^2 Pa, respectively, were studied using X-Ray photoelectron spectroscopy. The formation of surface sulfite at $T \geq 473$ K (the S $2p_{3/2}$ binding energy (E_b) is 167.5 eV) and surface sulfate at $T \geq 573$K (E_b = 169.2 eV) was observed in the reactions of Al_2O_3 and CeO_2 with SO_2. The formation of sulfates on the surface of CeO_2 occurred much more effectively than in the case of Al_2O_3, and it was accompanied by the reduction of Ce(IV) to Ce(III). The formation of aluminum and cerium sulfates and sulfites on model Pt/Al_2O_3 and Pt/CeO_2 catalysts occurred simultaneously with the formation of surface platinum sulfides (E_b of S $2p_{3/2}$ is 162.2 eV). The effects of oxygen and water vapor on the nature and yield of sulfur-containing products were studied.

HIGH-PRESSURE STUDIES OF CO ADSORPTION ON Pd(111) BY X-RAY PHOTOELECTRON SPECTROSCOPY AND SUM-FREQUENCY GENERATION

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J. Phys. Chem. B, 107(15) (2003) pp. 3522–3527.

High-pressure CO adsorption on Pd(111) was examined by X-Ray photoelectron spectroscopy (XPS) and vibrational sum frequency generation (SFG) from 200 to 400 K, and in a pressure range from 10^{-6} to 1 mbar. Even in the millibar regime both methods indicated that CO adsorbed in “regular” adsorption sites such as hollow, bridge, and on-top. By combination of XPS and SFG, a quantitative analysis of CO coverages at various pressures was performed. At high pressure, no CO structures different from those known from UHV studies were observed. Also, no indications of CO dissociation or carbonyl formation were found under the given experimental conditions, provided that the CO gas was sufficiently cleaned.

XPS STUDY OF METAL-SUPPORT INTERACTION IN Ru/MgO CATALYST FOR LOW-TEMPERATURE AMMONIA SYNTHESIS

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Chem. Sustain. Devel., 11(1) (2003) pp. 155–160.

The catalytic system Ru/MgO has been characterized by TEM and XPS in the Ru 3*d*, Cl 2*p* and O1*s* regions. It was shown, that the treatment of the sample with H_2 at 450°C leads to reduction of supported Ru (III, IV) chloride complexes to Ru metal crystallites of 2–5 nm in size (the surface atomic ratio Ru : Cl of reduced sample is 6.2). The shift of Ru 3*d* peak (279.5 eV) to lower bond energy (BE) found for Ru/MgO sample as compared with bulk Ru metal (280.2 eV) is proved to be due to the differential charging effect. The value of this effect was estimated by a comparison of the valence band spectrum of supported Ru particles with that of bulk Ru. Taking the differential charging into account, the "true" value BE of Ru $3d_{5/2}$ (280.5 eV) was determined. The shift of Ru 3*d* peak towards the higher BE values may indicate the electron-withdrawing effect of MgO surface to supported Ru particles.

AMMONIA FORMATION ON (Ru+Cs)/C CATALYSTS BY THE INTERACTION OF ADSORBED NITROGEN WITH HYDROGEN THAT DIFFUSED FROM THE BULK OF CESIUM-RUTHENIUM PARTICLES

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Kinet. Catal., 44(5) (2003) pp. 648–651.

The high-temperature α ($T_{\max}$ = 625 K) and β ($T_{\max}$ = 750 K) states of ammonia and α ($T_{\max}$ = 550–750 K), β ($T_{\max}$ =750-900 K), and γ ($T_{\max}$ > 900 K) states of hydrogen were detected on (Ru + Cs)/C catalysts for ammonia synthesis activated under the reaction conditions (P = 30 atm; T = 650 K; the initial pressure ratio $P_{N2}/P_{H2}=1/3$). A mechanism was proposed for the formation of ammonia as a result of the interaction of chemisorbed nitrogen with hydrogen that diffused from the bulk of cesium–ruthenium particles.

LOW-PERCENTAGE RUTHENIUM-CARBON CATALYSTS FOR SYNTHESIS OF AMMONIA

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Catal. Ind., 1 (2003) pp. 15–22.

The experimental results produced for the system ruthenium–alkali metal–carbon are given. The results allow the main mechanisms of changing activity in synthesis of ammonia to be found. The catalytic activity has been compared for the catalysts of different composition, and the operational features are established. The activity, characterized by ammonia content (in % vol.) in synthesized cesium-ruthenium catalysts which contain relatively low content of ruthenium (4 % wt.), is superior to that of well-known fused iron catalysts by an order of magnitude at the temperature < 350°C. The best cesium sample has activity of 16,8 % NH_3 in the mixture at T = 375 °C, P = 3,0 MPa, H_2:N_2 = 3:1, W = 2000 hr^{-1}, being superior to that of ruthenium-potassium samples the activity of best of which was 10,4 % NH_3 under the same conditions. By means of transferring to using mixture H_2:N_2 = 1:1 at the temperatures < 360°C, the synthesis temperature can be lowered by about 50 °C, as conformed to more than two-fold increase in yield of ammonia as compared with using the stoichiometric mixture of H_2:N_2 = 3:1. Ruthenium-cesium-carbon catalyst developed has a number of advantages useful for practical application.

INTERMETALLIC HYDRIDES $[TiFe_{0.95}Zr_{0.03}Mo_{0.02}]H_x$ ($0 \le x \le 2$): THE NATURE OF THE PHASE RESPONSIBLE FOR THE SELECTIVE REDUCTION OF CO_2

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Kinet. Catal., 44(2) (2003) pp. 165–174.

Based on data obtained by X-Ray diffraction and Mössbauer spectroscopy, it was concluded that tetragonal distortions appeared in the structure of cubic TiFe upon doping with Zr and Mo atoms and the intermetallide $TiFe_{0.95}Zr_{0.03}Mo_{0.02}$ is formed, which can absorb ~ 1 mol of H_2 per mole of the intermetallide. The heating of the hydrogen-saturated intermetallide in Ar to 185 ºC released ~ 0.80–0.82 mol of H_2 per mole of the intermetallide. This hydrogen was the constituent of cubic $[TiFe_{0.95}Zr_{0.03}Mo_{0.02}]H_{1.93}$ and orthorhombic $[TiFe_{0.95}Zr_{0.03}Mo_{0.02}]H$, which are the hydride phases of the parent $[TiFe_{0.95}Zr_{0.03}Mo_{0.02}]H_2$ hydride. The remainder of the hydrogen (~0.18 mol per mole of the intermetallide), which was released only at 700–920 ºC, entered the ν solution of nonstoichiometric TiH_{2-x}. EXAFS and XANES data indicate an increase in the signal intensity in the Ti–Ti direction and a decrease in electron density on titanium atoms for $[TiFe_{0.95}Zr_{0.03}Mo_{0.02}]H_{0.36}$. These results were interpreted in terms of a scheme according to which hydrogen atoms in an interstitial solid solution are arranged closer to titanium atoms and coordinated to them. It was found that a phase of $[TiFe_{0.95}Zr_{0.03}Mo_{0.02}]H_{0.36}$, which is a constituent of the ν solution, is responsible for the selective reduction of CO_2 to CO (90–98 %).

XAFS STUDY OF AN INTERMETALLIC $TiFe_{0.95}Zr_{0.03}Mo_{0.02}$ SYSTEM FOR CO_2 CONVERSION

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Nucl. Instrum. Methods Phys. Res., Sect. B,
199 (2003) pp. 216–221.

An intermetallic $TiFe_{0.95}Zr_{0.03}Mo_{0.02}$ system used for CO_2 conversion was studied by XAFS spectroscopy. The initial samples prepared by the skull-furnace method were exposed to the below treatments: (1) H_2 absorption (up to ~1 mol of H_2 per 1 mol of the initial sample); (2) H_2 thermal desorption (up to ~0.18 mol of H_2 at 180 °C in inert argon atmosphere); (3) hydrogen titration by CO_2 (at 350 °C for 4–6 h). For samples $[TiFe_{0.95}Zr_{0.03}Mo_{0.02}]H_{2x}$ ($x \leq 0.18$), the position of Ti-K edge shifts of about ~3 eV compared to that of the initial sample. From the XAFS studies of the modified $[TiFe_{0.95}Zr_{0.03}Mo_{0.02}]$ intermetallide, it is established that the interaction of dissolved hydrogen and titanium follows the donor–acceptor mechanism. Hydrogen atoms are located on the straight line connecting two titanium atoms. The one distance between a hydrogen atom and a titanium atom is less than 1.5 Å. It is proposed that the effect of strong binding of hydrogen in the $[TiFe_{0.95}Zr_{0.03}Mo_{0.02}]H_{2x}$ intermetallide at a molar concentration of absorbed hydrogen of 0.18 is associated with the formation of such binding.

MOBILITY AND REACTIVITY OF THE SURFACE AND LATTICE OXYGEN OF SOME COMPLEX OXIDES WITH PEROVSKITE STRUCTURE

V.A. Sadykov, N.N. Bulgakov, V.S. Muzykantov, T.G. Kuznetsova, G.M. Alikina, A.I. Lukashevich, Yu.V. Potapova, V.A. Rogov, E.B. Burgina, V.I. Zaikovskii, E.M. Moroz, G.S. Litvak, I.S. Yakovleva, L.A. Isupova, V.V. Zyryanov, E. Kemnitz*, S. Neophytides* (*Humboldt University, Berlin, Germany; **Institute of High Temperature Processes, Patras, Greece)

Mixed Ionic Electronic Conducting Perovskites for Advanced Energy Systems,
Eds N. Orlovskaya, N. Browning, Kluwer Academic Publishers, Boston/Dordrecht/London, 2003,
pp. 49–70.

Mobility and reactivity of the surface and bulk oxygen of perovskite-like mixed oxides including lanthanum manganite (I) and ferrite (II) systems modified by Ca (I,II) and fluorine (I), as well as some Co, Fe-containing complex perovskites known to be good mixed conductors were considered. Combination of thermal analysis data, dynamic and isothermal oxygen isotope exchange, O_2 TPD, isothermal pulse/flow samples reduction by CO, H_2 and CH_4 TPR, was applied to characterize the accessible surface/bulk oxygen mobility and reactivity. Comparison of these results with earlier obtained data on the real (defect) structure of these systems by TEM, EXAFS, XRD, FTIRS of lattice modes, SIMS allowed to elucidate factors determining the oxygen mobility and reactivity. Quantitative description of the experimental energetic spectrum of oxygen bound with regular and defect surface sites of perovskites was obtained by using semiempirical Interacting Bonds method with a due regard for the surface faces termination and relaxation. Analysis of the barriers for oxygen migration in the perovskite lattice by this method revealed pronounced effect of cation vacancies.

EFFECT OF LANTHANUM MANGANITE MODIFICATION BY CALCIUM AND/OR FLUORINE ON THE BONDING STRENGTH, MOBILITY AND REACTIVITY OF THE LATTICE AND SURFACE OXYGEN

V.A. Sadykov, T.G. Kuznetsova, A.V. Simakov, V.A. Rogov, V.I. Zaikovskii, E.M. Moroz, D.I. Kochubey, B.N. Novgorodov, V.P. Ivanov, S.N. Trukhan, G.S. Litvak, N.N. Bulgakov, V.V. Lunin*, E. Kemnitz** (*Moscow Lomonosov State University, Moscow, Russia; **Humboldt University, Berlin, Germany)

Mat. Res. Soc. Symp. Proc.,
V. 751, Z3.27.1.-6., 2003.

Ca and/or F-modified samples of lanthanum manganite have been prepared by Pechini method. The bulk structure of samples was characterized by TEM, EXAFS and XRD, while the surface composition was studied by SIMS. Thermal analysis, O_2 TPD, H_2 TPR and isothermal pulse/flow samples reduction by CO was applied to characterize the accessible surface/bulk oxygen mobility and reactivity. Reasonable description of the experimental energetic spectrum of the surface oxygen for various types of regular and defect surface sites on perovskite faces was achieved by using semiempirical Interacting Bonds Method in the slab approximation with a due regard for the different surface faces termination and relaxation. Fluorine was found to decrease the surface coverage by reactive weakly bound oxygen while increasing the bulk oxygen excess and mobility. Calcium generated reactive weakly bound oxygen forms while decreasing the oxygen excess in the lattice and converting regular M-O oxygen forms into bridging ones through migration to the surface.

MICROHETEROGENEOUS SOLID SOLUTIONS IN PEROVSKITES: FORMATION, MICROSTRUCTURE AND CATALYTIC ACTIVITY

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"Mixed Ionic Electronic Conducting Perovskites for Advanced Energy Systems",
Eds. N. Orlovskaya, N. Browning,
Kluwer Academic Publishers,
Boston/Dordrecht/London, 2003, pp. 137–156.

Influence of the point and extended defects on the steady-state catalytic activity of perovskites in deep oxidation processes is discussed.

REACTIONS OF Re^+, Re_2^+, ReO_x^+ (x=1-3) IONS WITH SMALL HYDROCARBON MOLECULES IN THE GAS PHASE

V.B. Goncharov

Russ. J. Phys. Chem.,
77(7) (2003) pp. 1103–1111.

Reactions of the Re^+ and Re_2^+ ions and the ReO_x^+ (x = 1–3) oxygen-containing ions with methane, propane, propylene, and cyclopropane were studied by ion cyclotron resonance. The formation of several organometallic ions, $Re(C_3H_6)^+$, $Re(C_3H_4)^+$, $Re_2(C_3H_6)^+$, and $Re_2(C_3H_4)^+$, including rhenium metallocarbene $ReCH_2^+$ and oxometallocarbenes $ReO_{x-1}CH_2^+$ (x = 2, 3) was observed. The upper and lower bounds for bond energies in these complexes were determined, namely, $111 > D_0(Re^+\text{-}CH_2) > 88.4$, $D_0(Re^+\text{-}C_3H_6) > 69$, $D_0(Re_2^+\text{-}C_3H_6) > 69$, $D_0(Re^+\text{-}C_3H_4) > 70.5$, $D_0(Re_2^+\text{-}C_3H_4) > 70.5$, $D_0(ReO^+\text{-}CH_2) > 110$, and $D_0(ReO_2^+\text{-}CH_2) > 118$ kcal/mol.

REACTIONS OF NEUTRAL AND CHARGED MOLYBDENUM OXIDE CLUSTERS WITH LOW-MOLECULAR-WEIGHT ALCOHOLS IN A GAS PHASE STUDIED BY ION CYCLOTRON RESONANCE

V.B. Goncharov

Kinet. Catal., 44(4) (2003) pp. 499–512.

A set of oxygen-containing molybdenum oxide clusters Mo_xO_y (x = 1-3; y = 1–9) was obtained with the use of a combination of a Knudsen cell and an ion trap cell. The reactions of positively charged clusters with C_1-C_4 alcohols were studied using ion cyclotron resonance. The formation of a number of organometallic ions, the products of initial insertion of molybdenum oxide ions into the C–O and C–H bonds of alcohols, and polycondensation products of methanol and ethanol were found. The reactions of neutral molybdenum oxide clusters Mo_xO_y (x = 1–3; y = 1–9) with protonated C_1-C_4 alcohols and an ammonium ion were studied. The following limits of proton affinity (*PA*) were found for neutral oxygen-containing molybdenum clusters: (MoO) < 180, (Mo_2O_4, Mo_2O_5, and Mo_3O_8) = 188±8, *PA*(MoO_2 = 202±5, *PA*(MoO_3, Mo_2O_6, and Mo_3O_9) > 207 kcal/mol.

CO-FREE METHYL FORMATE FROM METHANOL: THE CONTROL OF THE SELECTIVITY OF THE PROCESS ON Cu-BASED CATALYSTS

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Chem. Sustain. Devel., 11(1) (2003) pp. 189–195.

The influence of the structure and composition of precursor (which is used as support after treatment) and the structure of copper particles formed in the course of activation of copper containing catalysts by hydrogen on their catalytic properties in methanol dehydrogenation and reactivity towards hydrogen adsorption has been studied. The reactivity of catalyst towards hydrogen adsorption was investigated by means of Thermal Desorption Spectroscopy (TDS). Two catalysts preserving the structure of their precursor-oxide after reduction (CuZnSi and CuCr) and having strong bonds of metal particles with the surface are characterized by hydrogen adsorption at elevated temperatures. This type of adsorption is not observed for usual unsupported metal copper and for two other catalysts Cu/SiO_2 and Cu/Cr_2O_3. Methanol dehydrogenation proceeds via successive reactions $2CH_3OH = CH_3OOCH + 2H_2$ (I) and $CH_3OOCH = 2CO + 2H_2$ (II). The catalyst activity in reaction (II) greatly depends on the state of metal copper in the catalyst. It was assumed that catalyst activity in methyl-formate conversion to CO and H_2 and, hence, the selectivity of methanol dehydrogenation in respect to methylformate at moderate methanol conversion depends on the character of interaction between metal copper particles and catalyst oxide surface, which is determined by the composition and structure of oxide precursor.

ADSORPTION OF HYDROGEN ON REDUCED COPPER CHROMITE

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React. Kinet. Catal. Lett., 79(1) (2003) pp. 85–92.

Temperature programmed desorption and volumetric methods in static conditions were used to study hydrogen adsorption on the surface of metallic copper particles produced by the partial reduction of copper chromite $CuCr_2O_4$ with hydrogen. In the temperature range 300–573 K and in the range of medium surface coverages by hydrogen, the main state of adsorbed hydrogen reveals the heat of adsorption q = 78 kJ/mol and activation energy of adsorption Ea = 69 kJ/mol. In the temperature range 77–300 K, an adsorption state with lower heat and activation energy was found, indicating a non-uniformity of the copper surface within ca. 8 % of the total number of surface sites.

WATER CONDENSATION KINETICS ON A HYDROPHOBIC SURFACE

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Phys. Rev. Lett., 90(15) (2003) 156103 (4 pp.).

Employing thermal desorption spectroscopy, it has been shown that the effective probability of water condensation at low water vapor pressure on an octane film is much below unity at 100-120 K. This unusual finding is related to a small binding energy of H_2O monomers on octane (about 0.08 eV), requiring the formation of critical water clusters for condensation to occur. This results in strong temperature and impingement-rate dependencies of the water condensation rate and a non-linear uptake as a function of dose time. All these features are rationalized quantitatively or qualitatively by a kinetic model of water condensation.

INTERPRETATION OF ISOTOPE EXCHANGE DATA “WITHOUT TIME”: NONISOTHERMAL EXCHANGE OF DIOXYGEN WITH OXIDES

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Kinet. Catal., 44(3) (2003) pp. 319–322.

As a result of transformation of isotope-exchange rate equations (isotope-kinetic equations), a relationship was derived that does not contain time and universally relates the variables of isotope composition (an isotope-mechanistic equation). With the use of this relationship, mechanistic parameters that characterize atomic rearrangements can be determined from experimental data even in cases when the rate of exchange varied in the course of a process, for example, under nonisothermal conditions. The use of the proposed approach for the treatment of the results of dynamic thermal isotope exchange in the

O_2–$YBa_2Cu_3O_y$ and O_2–Pt/CeZrO systems demonstrated that the experimental data were excellently described by the theoretical equation derived in this work.

KINETICS AND MECHANISM OF 2,3,6-TRIMETHYLPHENOL OXIDATION BY HYDROGEN PEROXIDE IN THE PRESENCE OF TiO_2-SiO_2 AEROGEL

N.N. Trukhan, O.A. Kholdeeva

Kinet. Catal., 44(3) (2003) pp. 347–352.

The product and kinetics studies of 2,3,6-trimethylphenol (TMP) oxidation by 30% aqueous H_2O_2 in the presence of a heterogeneous catalyst, TiO_2-SiO_2 aerogel, are performed in an MeCN medium. The main reaction products are 2,3,5-trimethyl-1,4-benzoquinone and 2,2',3,3',6,6'-hexamethyl-4,4'-biphenol. The reaction is first-order in H_2O_2 and fractional order (1–0) in TMP. The reaction rate is proportional to the catalyst amount and depends on the water concentration in the reaction mixture in a complex manner. The results suggest the formation of an active intermediate on the titanium center. In this intermediate containing both a TMP molecule and the hydroperoxide group, inner-sphere one-electron oxidation of TMP occurs to give the phenoxyl radical.

H_2O_2-BASED SELECTIVE OXIDATIONS OVER TITANIUMSILICATES OF SBA-15 TYPE

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Microporous Mesoporous Mater.,
59(2-3) (2003) pp. 73–84

Hexagonally packed mesostructured titaniumsilicates of the SBA-15 type have been prepared in moderately-acidic aqueous media starting from sodium disilicate $Na_2Si_2O_5$, $Ti(SO_4)_2$, and olefin oxide co-polymer of the Pluronic type (P123) as a template. Structure-texture parameters of the synthesised materials were characterised by using X-Ray diffraction and nitrogen adsorption techniques. The titanium state in the silicate matrix was characterised by DR-UV, IR, Raman spectroscopy and XPS. Catalytic properties of the new titaniumsilicates were tested in oxidations with aqueous H_2O_2 using methyl phenyl sulfide and 2,3,6-trimethylphenol as model substrates and compared with catalytic properties of TS-1 and Ti-MMM (titaniumsilicates of the MCM-41 type). The structure of the Ti-SBA-15 materials, by contrast to Ti-MMM catalysts, was proved to be hydrolytically stable towards aqueous H_2O_2. The catalytic activity of Ti-SBA-15 is considerably lower compared to the catalytic activity of Ti-MMM most likely due to lower titanium dispersion and higher wall-thickness of the former material, which makes a part of titanium sites unavailable for reactants.

OXIDATIVE ADDITION OF HYDROGEN IN THE "REDUCED" Mo/Al_2O_3 CATALYSTS

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React. Kinet. Catal. Lett.,
80(1) (2003) pp. 97–103.

An X-Ray photoelectron spectroscopy study of Mo/Al_2O_3 catalysts prepared via $[MoV_2O_4(C_2O_4)_2(H_2O)_2]^{2-}$ complexes showed that after heating the catalysts with hydrogen in the spectrometer chamber, the position of the Mo3d line shifted to higher values of binding energy. This shift is interpreted as oxidative addition of hydrogen to the surface Mo species. A similar phenomenon was observed for a CO treated catalyst. A temperature-programmed desorption study has shown that hydrogen is strongly bounded to Mo and can only be removed from the catalysts at temperatures as high as 500°C.

THE REACTION MECHANISM OF SELECTIVE CATALYTIC REDUCTION OF NITROGEN OXIDES BY HYDROCARBONS IN EXCESS OXYGEN: INTERMEDIATES, THEIR REACTIVITY, AND ROUTES OF TRANSFORMATION

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Kinet. Catal., 44(3) (2003) pp. 379–400.

The main features of the mechanism of selective reduction of nitrogen oxides by hydrocarbons (methane, propane, and propylene) in excess oxygen catalyzed by systems containing transition metal cations are considered. A combination of steady-state and non-steady-state kinetic studies, *in situ* Fourier-transform infrared (FTIR) spectroscopy, temperature-programmed desorption, and theoretical analysis of bond strengths and spectral data for adsorption complexes made it possible to determine reliably that surface nitrate complexes are key intermediates at real temperatures of catalysis. The rate-limiting step in these reactions includes the interaction of these complexes with hydrocarbons or their activated forms. Factors are considered that determine the structure, bond strength, and routes of nitrate complexes transformations under the action of hydrocarbons. Mechanistic schemes are proposed for the reaction of various types of hydrocarbons in which the determining role belongs to the formation of organic nitro compounds in a rate-limiting step. Their further fast transformation with the participation of surface acid sites resulting in the formation of ammonia, which is a highly efficient reducing agent, though not limiting the whole process, but determines nevertheless both the selectivity to the target product, molecular nitrogen, and the selectivity of hydrocarbon consumption for nitrogen oxide reduction.

OSCILLATIONS IN PARTIAL OXIDATION OF METHANE TO SYNGAS OVER SUPPORTED MIXED OXIDES PROMOTED WITH Pt

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Chem. Sustain. Devel., 11(1) (2003) pp. 263–270.

Ni, Pt, lanthanum nickelate with and without Pt supported on corundum carrier either pure or promoted with CeO_2–ZrO_2 were tested in partial methane oxidation (POM) to synthesis gas under conditions (high temperature, short contact time, highly diluted gas mixture, small catalyst grains) providing studying of the intrinsic kinetics. The phase composition and reducibility of catalysts were characterized with XRD and TPR technique. The influence of catalyst composition on the catalyst performance has been studied. The self-sustained oscillations of methane conversion and products concentration have been observed. The nature of those oscillations is discussed taking into account the intrinsic properties of the catalysts clarified with TPR and XRD.

OXIDATIVE DEHYDROGENATION OF BUTANE OVER NANOCRYSTALLINE MgO, Al_2O_3, AND VO_x/MgO CATALYSTS IN THE PRESENCE OF SMALL AMOUNTS OF IODINE

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J. Catal., 218(2) (2003) pp. 438–446.

High surface area nanocrystalline MgO, Al_2O_3, $MgO{\cdot}Al_2O_3$, commercial MgO, and a series of 10 % V/MgO samples were used as catalysts in one-step selective oxidative dehydrogenation of butane to butadiene in the presence of oxygen and iodine. Molecular iodine shifts the equilibrium of the dehydrogenation reactions to the right and makes it possible to achieve high butane conversion with high selectivity to butadiene. When excess oxygen is present in the feed, iodine is successfully regenerated and can be recycled. Butadiene selectivity as high as 64 % has been achieved in the presence of small amounts of iodine (0.25 vol %) over a vanadia–magnesia catalyst at 82 % butane conversion. The best performance was observed over a catalyst containing the magnesium orthovanadate phase.

KINETICS OF FREE RADICAL GENERATION IN THE CATALYTIC OXIDATION OF METHANOL

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Kinet. Catal., 44(4) (2003) pp. 536–546.

The formation of free radicals over the surface of platinum-containing catalysts in the methanol oxidation reaction depending on the temperature, the composition of the reaction mixture, and the procedure used for introducing platinum was studied by the matrix isolation method technique. The nature and transformations of surface intermediates depending on the temperature and the presence of oxygen in the gas phase were studied by Fourier transform IR spectroscopy. The main surface intermediate was the methoxy group. The following three types of these groups were stabilized in alumina-based catalysts: (I) CH_3O–Al_{oct} (ν_s(C–H) = 2806 cm^{-1}), (II) CH_3O–Al_{tetr} (ν_s(C–H) = 2825 cm^{-1}), and (III) $CH_3O < (Al)_2$ (ν_S(C–H) = 2845 cm^{-1}, δ_{as}(C–H) = 1460 cm^{-1}, δ_s(C–H) = 1440 cm^{-1}, $r_{||}$ (CH_3) = 1185 cm^{-1}, and ν (C–O) = 1095 cm^{-1}). At the same time, isolated methoxy groups (ν_{as}(C–H) = 2997 cm^{-1}, ν_{as}(C–H) = 2959 cm^{-1}, ν_s(C–H) = 2857 cm^{-1}, and δ(CH_3) = 1450 cm^{-1}) and hydrogen-bonded groups

(ν(O–H) = 3400–3550 cm^{-1}), which resulted from chemisorption at siloxane bridges, were stabilized in silica gel–based catalysts. It was found that CH_3O' and CH_3OO' radicals were formed only over the surfaces of pure supports (SiO_2 and Al_2O_3) and their mechanical mixtures with platinum. The total concentration of radicals was described by an extremal function of the composition of reactants, whereas the relative concentration depends on the nature of the support. This is conceivably due to the effect of coordinatively unsaturated cations of the support, which are formed by dehydroxylation in the course of catalyst pretreatment. An increase in the rate of formation of gas-phase radicals on mixed catalysts was explained by special properties of the platinum/support interface region, at which surface intermediates were formed in superequilibrium concentrations under reaction conditions.

AMMOXIDATION OF METHYLPYRAZINE OVER VANADIUM-TITANIUM CATALYSTS MODIFIED BY ALKALI ADDITIVES

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React. Kinet. Catal. Lett.,
78(2) (2003) pp. 355–363.

Vanadium-titanium catalysts modified with sodium or potassium additives (1-15 wt.% of Me_2O) have been studied in methylpyrazine ammoxidation. Introduction of the additives results in a decrease in the activity and selectivity of the catalysts due to formation of low-active phase - bronzes (MeV_6O_{15}) and vanadates (α-$NaVO_3$, KVO_3 and $K_3V_5O_{14}$). The active sites of the modified samples, similar to those in the V-Ti-O catalyst, are found to be V^{5+} cations strongly bound to TiO_2 and located in a significantly distorted octahedral oxygen environment.

AMMOXIDATION OF METHYLPYRAZINE OVER PHOSPHORUS-MODIFIED VANADIUM-TITANIUM CATALYSTS

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O.B. Lapina, A.A. Vlasov, L.S. Dovlitova

React. Kinet. Catal. Lett.,
79(1) (2003) pp. 165–173.

Vanadium-titanium catalysts modified with phosphorus additives (1-15 wt. % of P_2O_5) have been studied in methylpyrazine ammoxidation. Introduction of high amounts of the additive ($\geq$10 wt. % of P_2O_5) results in a decrease in activity and selectivity of the catalysts due to formation of low active phase - a ternary compound with the component ratio V:P:Ti $\approx$ 1:1:1 with only one type of slightly distorted tetrahedral vanadium (5+) bound via oxygen to phosphorus (5+). The nature of the active sites of the samples modified with 1-5 wt. % of P_2O_5, similarly to that in the V-Ti-O catalyst, was found to include the V^{5+} cations strongly bound with TiO_2 and located in the significantly distorted octahedral oxygen environment.

BENZENE HYDROGENATION ON SULFIDE CATALYST UNDER UNSTEADY-STATE CONDITIONS

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A.N. Startsev

React. Kinet. Catal. Lett.,
78(2) (2003) pp. 389–395.

A kinetic model of benzene hydrogenation on a sulfide hydropurification catalyst (Ni, Mo)/Al_2O_3 has been developed. The model describes well the experimental data obtained under nonsteady-state conditions and relies on the assumption that the catalyst surface contains only one type of active sites, i.e., Ni atoms in the sulfide bimetallic complex, and makes allowance for the transition of active sites into inactive sites.

WATER DENITRIFICATION OVER CATALYTIC MEMBRANES: HYDROGEN SPILLOVER AND CATALYTIC ACTIVITY OF MACROPOROUS MEMBRANES LOADED WITH Pd AND Cu

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Catal. Today, 82(1-4) (2003) pp. 49–56.

Mono- and bimetallic catalytic membranes were prepared via deposition of Pd and Cu onto macroporous polymeric membrane. The membranes were employed to catalyze the reaction of nitrate ions reduction by hydrogen in water. Monometallic Pd- and Cu-loaded membranes were poorly active in the reaction, while bimetallic (Pd+Cu)-loaded membranes exhibited high catalytic activity. Combination of monometallic Pd- and Cu-loaded membranes in one stack resulted in high catalytic activity, similar to that of bimetallic (Pd+Cu)-loaded membranes. The results of this study provide experimental support for a hypothesis on hydrogen spillover as a part of the molecular mechanism of nitrate ions reduction by hydrogen in water over palladium–copper catalytic system.

STUDIES ON THE PHENOL WET PEROXIDE OXIDATION IN THE PRESENCE OF SOLID CATALYSTS

O.P. Pestunova, O.L. Ogorodnikova, V.N. Parmon

Chem. Sustain. Devel., 11(1) (2003) pp. 227–232.

The comparative study of Fe-, Mn- and Cu-oxide catalysts supported on α-Al_2O_3, TiO_2, CeO_2 and pure graphite-like porous carbon Subunit in the catalytic wet phenol oxidation by hydrogen peroxide in a stirred batch reactor at 90°C was performed. The Fe-containing samples supported on α-Al_2O_3 are sufficiently active and most stable and selective in respect to the CO_2 evolution. Cu-containing catalysts are most active, Fe-containing catalysts appear to be much more stable and ecologically benign. The pure Subunit has shown an appreciable activity and highest selectivity in respect to CO_2. Hydroquinone and pyrocatechol have been found in the liquid phase as intermediates of the oxidation. Kinetics of the change of the phenol, hydrogen peroxide as well as intermediates concentration has been recorded. The oxidation of phenol over Subunit is assumed to occur via a mechanism, which is different from that for the oxide catalysts.

THE INFLUENCE OF THE DENSITY OF SUPERCRITICAL WATER ON THE RATE CONSTANT FOR THE DEHYDRATION OF ISOPROPANOL

V.I. Anikeev, A. Yermakova

Russ. J. Phys. Chem., 77(2) (2003) pp. 211–214.

A mechanism of the dehydration of 2-propanol and of the back reaction of the hydration of propylene in supercritical water was suggested; the mechanism corresponded to that of acid catalysis in solutions. The reaction rates in both directions were shown to be directly proportional to the concentration of the corresponding reagents and the H_3O^+ ions, which played the role of a homogeneous catalyst. It was also shown that a sharp increase in the concentration of H_3O^+ caused by increasing the density (pressure) unambiguously correlated with changes in the experimental rate constants for the pseudo-first-order reactions depending on the parameters specified above. The density-independent (pressure-independent) rate constants for bimolecular reactions were determined.

MECHANISMS OF IRON ACTIVATION ON Fe-CONTAINING ZEOLITES AND THE CHARGE OF α-OXYGEN

E.V. Starokon, K.A. Dubkov, L.V. Pirutko, G.I. Panov

Top. Catal., 23(1-4) (2003) pp. 137–143.

According to the previous Mössbauer data α-sites formation at the activation of Fe-containing zeolites is accompanied by irreversible "self-reduction" of the iron, proceeding without participation of an external reducing agent. Reduced Fe^{2+} ions are inert to O_2, but reversibly oxidized to Fe^{3+} by N_2O, generating the α-oxygen species, Oα, which provide selective oxidation of hydrocarbons.

In this work, the mechanism of α-sites formation was studied via quantitative measurement of dioxygen amount desorbed into the gas phase at the step of "self-reduction". A prominent role of the zeolite matrix chemical composition has been revealed. For example, with zeolites of Al-Si composition (FeZSM-5 and Fe-β), heating to 900 °C in a closed vacuum space leads to irreversible evolution of O_2, which is accompanied by immediate formation of α-sites. Similar heating of B-Si and Ti-Si zeolites also leads to dioxygen evolution; however, this evolution is reversible and not accompanied by formation of α-sites. Activation of these zeolites occurs only in the presence of water vapor. Stoichiometric measurements showed that in terms of charge one regular O^{2-} ion, removed at the activation, is equivalent to two α-oxygen atoms. So, α-oxygen is identified as an ion-radical species $O_{\alpha}^{-\bullet}$, whose unique oxidation properties still distinguish it from the generally observed $O^{-\bullet}$ radicals.

The mechanism of α-sites formation is proposed, in which the process of strong chemical stabilization of reduced Fe^{2+} atoms in the zeolite structure is a key step, making impossible the reoxidation of the iron with O_2.

SURFACE STATE OF A SILVER CATALYST FOR ETHYLENE GLYCOL OXIDATION

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Kinet. Catal., 44(3) (2003) pp. 408–413.

The surface state of electrolytic silver before and after treatment with a reaction mixture in the course of ethylene glycol oxidation to glyoxal was studied using X-Ray photoelectron spectroscopy and scanning electron microscopy. It was found that electrophilic forms of adsorbed oxygen, which participate in the selective conversion of ethylene glycol, were formed on the surface of electrolytic silver crystals under exposure to oxygen under conditions similar to catalytic process conditions. The treatment of the catalyst with a reaction mixture resulted in the formation of filamentous carbon deposition products. A mechanism of formation of carbon-containing products was proposed.

DEEP OXIDATION OF FLUORINATED HYDROCARBONS IN MOLTEN CATALYSTS

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Eurasian Chem.-Tech. J.,
5(2) (2003) pp. 137–143.

The oxidation of fluorine-containing organic substances: fluorocarbon liquid M-1, fluorinated alcohol $H(CF_2)_8CH_2OH$, and powder polytetrafluoroethylene with air has been studied in melts: NaOH; 43 mol. % LiCl – 33 mol. % NaCl – 24 mol. % KCl (eutectic mixture); (LiCl-NaCl-KCl)eutec. + 10 mass. % V_2O_5; (LiCl-NaCl-KCl) eutec. + 15 mass. % V_2O_5; 56 mol. % Na_2CO_3 – 44 mol. % K_2CO_3 (eutectic), (Na_2CO_3 – K_2CO_3)eutect. + 15 mass. % V_2O_5, and $K_3V_5O_{14}$.

The compositions of the melts have been examined by GC, DTA, chemical analysis and XRD, and they have been shown to change during the reaction, depending on the composition and partial pressure of the gaseous products over the melt surface. The alkali metal chloride melt containing 15 mass. % V_2O_5 has been found to be most stable to the action of fluorine compounds.

Possibility of deep oxidation of fluorine-containing organic substances in melts based on hydroxides, carbonates and chlorides of alkali metals doped with oxides of vanadium has been proved. The process of deep oxidation of fluorinated hydrocarbons is accompanied by formation of an equilibrium mixture containing hydroxides, carbonates, chlorides and fluorides of alkali metals, as well as their vanadates, if V_2O_5 additive is used. The relative amounts of these substances in molten systems are determined by the partial pressure of oxygen, CO_2 and water vapor.

Application of Physicochemical Methods for Characterization of Catalysts, Supports, Synthesized Substances and Materials

STRUCTURE OF GLASSES IN THE Na_2SO_4-P_2O_5-H_2O SYSTEM

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Glass Phys. Chem., 28(1) (2002) pp. 1–4.

The structure of sulfate–phosphate glasses is investigated by high-resolution ^{31}P solid-state nuclear magnetic resonance with magic-angle sample spinning (^{31}P MAS NMR spectroscopy). The structure parameters that account for the number of different types of phosphorus–oxygen structural units involved in the glass network are determined, and the main structural units of the glasses under investigation are revealed. The role of H_2O and Na_2SO_4 as modifiers of the structural network of sulfate–phosphate glasses is clarified.

^{1}H AND ^{29}Si-MAS NMR CHARACTERIZATION OF SILICATE FIBERGLASS SUPPORTS

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Phys. Chem. Chem. Phys.,
5(12) (2003) pp. 2686–2691.

The structural properties of alumina–sodium–silicate fiberglass (S) and microporous silica–alumina fiberglass supports (CCB18 and CCB20) were investigated using solid state NMR. Structural changes of samples of S as a result of partial extraction of Na with acid treatment were explored. Strongly and weakly hydrogen-bonded hydroxyls with non-uniform distribution of hydrogen bond strengths were revealed. Decreasing of Na concentration is followed with partial polymerization of the glass framework and hydroxylation of the surface. Deuterium exchange and the thermal dependence of the dehydration of silica–alumina fiberglass (CCB18 and CCB20) were monitored using ^{1}H and ^{29}Si MAS technique in order to classify surface hydroxyl groups. These samples were prepared by full extraction of Na from alumina–sodium–silicate fiberglass materials similar to S. At least four types of hydroxyl groups were revealed for both samples: internal isolated accessible silanols (2.65 ppm), internal silanols (6.7 ppm and 3.7 ppm) with low accessibility, molecular water displaying broad resonance at 5±1 ppm. Spin–spin relaxation times T_2 were measured for these silanol groups using a standard echo sequence. The full content of water and silanol groups were determined.

^{51}V 3QMAS NMR AND ITS APPLICATION FOR THE STUDIES OF VANADIA BASED CATALYSTS

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"Magnetic Resonance in Colloid and Interface Science",
Eds. J. Fraissard and O. Lapina, NATO ASI Series,
Kluwer Academic Publishers, The Netherlands, 2002,
pp. 355–365.

Vanadia based catalysts are widely used in industry for many purposes such as, selective oxidation of hydrocarbons, reduction of nitrogen oxides with ammonium (SCR), and cleaning of flue gases. Despite they have been extensively investigated by modern physico-chemical techniques, complexity of the catalytic systems and technical limitations have prevented a clear view of the active species structure.

During the last few years, the Multi-Quantum Magic Angle Spinning (MQMAS) was largely used for precise characterization of local structure of quadrupolar nuclei with half integer spin. Simple in realization and very effective in resolution this method has became very popular, and spectacular results have been obtained with a number of nuclei (aluminum, sodium, rubidium, boron). However, it is commonly admitted that small value of quadrupolar moment and large value of chemical shielding anisotropy are a limitation to MQMAS and, in particular, prevent its application to vanadium nucleus.

It is demonstrated that MQMAS technique can be successfully applied to vanadium nucleus and used for the study of supported vanadia catalysts.

SYNERGY PHENOMENON IN BULK RUTHENIUM-VANADIUM MIXED SULFIDES: ^{51}V NMR AND ESR STUDIES

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"Magnetic Resonance in Colloid and Interface Science",
Eds. J. Fraissard and O. Lapina, NATO ASI Series,
Kluwer Academic Publishers, The Netherlands, 2002,
pp. 531–537.

For a better protection of the atmospheric environment, catalytic hydroprocessing will become increasingly important in the years to come. This is due to the need for light distillates simultaneously with a stricter environmental legislation. Since the works of Chianelli and Harris, it is well known that mixing two transition metal sulfides (TMS) allows developing higher activity than the ones exhibited by pure compounds in hydrotreatment reaction. From this point of view, the CoMo and NiMo conventional catalysts have been widely used. So far, an explanation for such a synergism is still matter of debate and understanding of the synergy phenomenon becomes fundamental. Previous results show that, rather a structural effect, we are in presence of electronic effect, which changes noticeably the environment of active site. As an example, all the iron-based mixed sulfides present, in Mossbauer spectra, only one iron species, which is Fe^{2+} low spin. Moreover, it is showed that there is a linear correlation between the hyperfine field distribution and the activity of vanadyloctaethylporphyrine hydrodeporphyrinisation. The evolution of the HPF at room temperature for different relative concentration of iron is due to the changes in the density of state of the d electrons at the Fermi level. Magnetic resonance appears as one of the technique that can give a part of the response. As ruthenium sulfide is one of the best catalyst for hydrodesulfurisation (HDS) and V is also a good candidate for the synergy phenomenom, bulk

RuV mixed sulfides were chosen to performed a study by solid state NMR and ESR.

SOLID-STATE ^{51}V NMR FOR CHARACTERIZATION OF VANADIUM-CONTAINING SYSTEMS

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Catal. Today, 78(1–4) (2003) pp. 91–104.

This overview paper includes both published and original data of the current state of the field of ^{51}V NMR in solid-state chemistry. Advantages and shortcomings of different NMR techniques in their applications to vanadium are discussed on the examples of their application to various vanadia based systems (including individual highly crystalline compounds, solid solutions, glasses, catalysts). New correlations between local structure of vanadium atoms and NMR parameters allowing to discriminate at least seven different types of vanadium sites (tetrahedral sites of Q^0, Q^1 and Q^2 types; trigonal pyramids of 3=1 and 3=2 (V_2O_5 like) types; tetragonal pyramids of 4=1, 4=2 types) are proposed. It is demonstrated that competent combination of different NMR approaches permits now not only to describe different vanadium sites in highly crystalline and amorphous materials, but also to insight into the structural aspects of disorder in crystallinity as well as to reveal the behavior of different functional groups at elevated temperatures. The influence of low valence vanadium atoms on ^{51}V NMR spectra is also discussed.

CORRELATION OF ^{51}V NMR PARAMETERS WITH LOCAL ENVIRONMENT OF VANADIA SITES

D.F. Khabibulin, A.A. Shubin, O.B. Lapina

"Magnetic Resonance in Colloid and Interface Science",
Eds. J. Fraissard and O. Lapina, NATO ASI Series,
Kluwer Academic Publishers, The Netherlands, 2002,
pp. 537–546.

Vanadium oxide based catalysts are widely used in industry. Generally, the activity of heterogeneous catalysts is determined by the structure of active centers. For characterization of active vanadium species by ^{51}V NMR spectroscopy the knowledge of correlation between parameters of NMR spectra and local structure of vanadium sites is necessary. It may be found successfully for individual vanadium compounds with known structure. Earlier, the correlation between the anisotropy of the chemical shielding tensor and the local environment of vanadium sites was demonstrated, but for the detailed characterization of these sites the knowledge of other ^{51}V NMR parameters is also necessary. Recently, SATRAS – the numeric analysis of spinning side bands intensities in MAS NMR spectra, was proposed by Skibsted et al. This analysis allows the determination of magnitudes and relative orientation of ^{51}V chemical shielding (CS) and quadrupling coupling (QC) tensors. In earlier reports all eight parameters of ^{51}V NMR spectra were presented with high accuracy for some orthovanadates and alkali metal metavanadates, as well as for the series of divalent metal metavanadates and pyrovanadates.

In this study SATRAS approach was used in order to obtain ^{51}V NMR parameters for a number of vanadates and other vanadium compounds. This investigation is devoted to a search for more accurate correlations between the anisotropy of chemical shielding tensor and local environment of vanadium. In addition, correlations between vanadium local environment and some other ^{51}V NMR spectrum parameters were also examined.

HIGH-TEMPERATURE NMR STUDIES OF IONIC-LIQUID CATALYSTS

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"Green Industrial Application of Ionic Liquids",
Eds. R.D. Rogers et al, NATO ASI Series,
Kluwer Academic Publishers, The Netherlands, 2003,
pp. 85–104.

The number of "green" applications of ionic liquids (ILs) is progressively growing in recent years due to the chemical industry reorientation, including catalysis, towards environmentally friendly processes. Sulfuric acid production using silica-supported alkali metal pyrosulfate-vanadium oxide catalyst ($M_2S_2O_7$-V_2O_5, hereinafter M = Na, K or Cs) was the first prominent application of an IL system in catalysis. SO_2 oxidation to SO_3 is carried out at high temperatures, where the active component of the catalyst is a melt. Today, similar IL systems are used in the processes of flue gas purification, and the technological benefits are recognised worldwide. A recently discovered promising method for the catalytic epoxidation of olefins with supported alkali nitrate melts exemplifies another breakthrough application of catalysis by IL. Since the IL systems development demands a detailed understanding of their properties, several modern measuring techniques are used for their characterization. Among them nuclear magnetic resonance (NMR) spectroscopy holds a remarkable position, since it is one of the main analytical techniques for the study of liquids. NMR spectroscopy is widely used to investigate different physico-chemical aspects of multicomponent aqueous and non-aqueous solutions. Regarding the IL systems, NMR spectroscopy is applied mostly at room or close-to-room temperatures. There are only a few studies of high-temperature melts of inorganic salts using NMR spectroscopy, though such systems are of great importance for modern catalysis. First of all this can be explained by the technical difficulties involved. In the present report, the use of high temperature NMR techniques for studying ionic-liquid catalysts such as $M_2S_2O_7$-V_2O_5 and $MHSO_4$-V_2O_5 systems is demonstrated, and recent results obtained for molten alkali metal nitrate catalysts are shown.

NUCLEAR MAGNETIC RESONANCE OF DONOR ATOMS AS A TOOL FOR DETERMINATION OF THE STRUCTURE OF PLATINUM METAL COMPLEXES IN SOLUTIONS

M.A. Fedotov

Russ. Chem. Bull., 52(4) (2003) pp. 781–794.

Data on the NMR spectroscopy of C, N, O, Si, P, and Sn donor atoms of platinum metal complexes in solutions are surveyed. The chemical shift of a donor atom mainly depends on the ligand in the trans-position (due to the trans-effect). The chemical shift of a donor atom on a particular coordinate of the complex (coordinate shift, CSh) is an attribute of this coordinate and can be used to identify such a coordinate in platinum metal complexes and to determine the structures of complexes. Based on the known data, CSh diagrams were composed for ^{1}H, ^{13}C, ^{14}N, ^{17}O, ^{19}F, ^{31}P, and ^{119}Sn. Examples of using the CShs for determining the structures of platinum metal complexes in solutions are presented.

POSSIBILITIES OF MULTINUCLEAR NMR IN DETERMINATION OF ACIDITY OF HETEROPOLY ACID SOLUTIONS

M.A. Fedotov, G.M. Maksimov, S.V. Ignashin

Russ. J. Inorg. Chem.,
47(12) (2002) pp. 1867–1873.

The ^{14}N and ^{13}C NMR parameters of the acidity indicator *ortho*-nitroaniline (*o*-NA) and the ^{14}N and ^{17}O NMR parameters of substrates in solutions of some acids and heteropoly acids (HPA) have been measured. The ^{14}N and ^{13}C NMR parameters of Hammet acidity indicators and the ^{14}N and ^{17}O NMR parameters of anions and a solvent depend on the acidity of a solution. The NMR signals of the amino nitrogen atom and the carbon atom bearing the amino group are most sensitive. Comparison of the NMR parameters of the Hammet indicator *o*-NA in solutions of acids and HPAs shows that the interaction of HPAs with *o*-NA, which is not related to acidity, additionally contributes to the NMR parameters of *o*-NA in HPA solutions. It has been shown that the acidity of a water-containing solution can be estimated based on the ^{17}O NMR parameters of water.

DEUTERIUM SOLID-STATE NMR STUDY OF THE DYNAMIC BEHAVIOR OF DEUTERONS AND WATER MOLECULES IN SOLID $D_3PW_{12}O_{40}$

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J. Phys. Chem. B,
107(47) (2003) pp. 12330–12337.

The mobility of water molecules and protons of the deuterated analog of solid 12-tungstophosphoric acid, $H_3PW_{12}O_{40}\cdot nH_2O$ (HPA) (n = 5.5 and 0.1) has been characterized by deuterium solid state NMR. Analysis of the ^{2}H NMR line shape and spin-lattice relaxation times allowed to characterize the proton and water dynamics in HPA, at different water contents, in the temperature range 103-383 K. At 163-193 K and for $n = 5.5$, an intramolecular motion corresponding to reorientations by 180° flips around the C_2 axis of water in the $[H_5O_2]^+$ ion has been detected, the proton being probably immobile. At temperatures above 313 K, both water and proton become involved in fast rotation around the C_3 axis of the formed hydroxonium ion. The rotation is performed on a time scale of 30-50 ns with an activation energy E_a of 8.5 kJ/mol. For n = 0.1, three dynamically different species can be distinguished: mobile protons, mobile hydroxonium ions and immobile protons. Mobile protons are weakly bonded to polyanions and move fast with a characteristic time of a few picoseconds and E_a = 8.6 kJ/mol. Hydroxonium ions move more slowly than protons, but still fast: time scale of a few nanoseconds and E_a = 17.6 kJ/mol. The characteristic time for immobile protons is much greater than a few microseconds.

DYNAMICS OF *N*-HEXANE INSIDE SILICALITE, AS STUDIED BY ^{2}H NMR

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J. Phys. Chem. B, 107(29) (2003) pp. 7095–7101.

Perdeuterated *n*-hexane, adsorbed in silicalite, has been found to exhibit a ^{2}H NMR spectrum which represents a superposition of three Pake–powder patterns. Two Pake-powder patterns with the spectral parameters (quadrupole constants C_Q and asymmetry parameter η) C_Q = 23.5 kHz and $\eta = 0$ and C_Q = 30.1 kHz and $\eta = 0$ belong to different methylene groups and one powder pattern with C_Q = 7.0 kHz and η = 0.7 arises from the methyl groups. The observed line shapes have been concluded to arise from the fast anisotropic translational and rotational motions of the alkane in the silicalite channels. The reduction of the quadrupole constants compared to that in rigid *n*-hexane and the appearance of an asymmetry parameter for the methyl groups have been interpreted in terms of three modes of motion exhibited by *n*-hexane inside the channel system: (a) rotation of the molecule about the channel axis; (b) trans/gauche conformational isomerization around nonterminal C-C bonds and rotation of the methyl groups around terminal C-C bonds; (c) fast interchange of the adsorbed molecules between both straight and zigzag channels and along zigzag channels with an effective angle Θ~90° between adjacent sites of the molecule location during successive jumps. The percentage of trans/gauche conformations is estimated to be 78/22, which exceeds that in gas phase or liquids. This demonstrates that constraining effects of the narrow silicalite pore walls retain the molecules in a more elongated conformation compared to that in a gas phase or liquid. The rotation of a methyl group around a terminal C-C bond has been estimated to occur with a characteristic time of ~40 ps at 300 K and an activation energy of 9.4 kJ/mol. The reorientation of methylene groups, corresponding either to conformational isomerization or to translational diffusion, occurs one order of magnitude slower with a characteristic time of ~300 ps and an activation energy of 7.5 kJ/mol.

COMPARISON OF THE DYNAMICS OF N-HEXANE IN ZSM-5 AND 5A ZEOLITE STRUCTURES

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Eur. Phys. J. E, 12(3) (2003) pp. 345–349.

The translational and rotational dynamics of *n*-hexane adsorbed in ZSM-5 and 5A zeolites has been studied by neutron scattering and deuterium solid state NMR, at various temperatures. The dynamics of *n*-hexane is quite different in the two zeolites. In the ZSM-5 structure, the molecule sits in channel segments, the energy barrier between adjacent adsorption sites is small and fast anisotropic motions are observed. In the 5A zeolite, the molecule is adsorbed in α-cages; the barrier between adjacent cages is larger so that the molecule spends a longer time exploring the volume of an α-cage, leading to a more isotropic motion. The diffusion coefficient of the molecule is reduced by more than 4 orders of magnitude in 5A zeolite compared with ZSM-5.

CARBONYLATION – HETEROGENEOUS

A.G. Stepanov

Encyclopedia of Catalysis, Ed. I.T. Horvath, Willey-Interscience, V. 2, 2003, pp. 71–104.

In this article basic heterogeneous carbonylation catalysts known to date and their application for the conversion of the particular olefins, alcohols, alkanes into carboxylic acids, ketones, aldehydes, etc., have been described. Two approaches for the design of heterogeneous catalysts are considered. The first one is a direct heterogenization of high efficiency homogeneous carbonylation catalysts used in the Reppe reaction. This approach is based on the three ways of heterogenezation of homogeneous metal complexes: by anchoring on polymers, amorphous oxides or zeolites, and inert carboneous supports. These metal- or metal-complex-supported catalysts usually require alkyl halide promoters. The other approach consists of using the analogues of the liquid strong-acid catalysts in the Koch reaction, that is, the pure solid acidic catalysts, such as acidic zeolites, heteropoly acids, acidic ion-exchanged resins, and sulfated zirconias. Analysis of the carbonylation catalysts is given on the basis of the type of support used in the first approach and the conditions for carbonylation performance (liquid phase or vapor phase carbonylation) in both approaches.

MODEL Ag/HOPG AND Ag/ALUMINA CATALYSTS: STM AND XPS STUDY

A.V. Nartova, R.I. Kvon

Chem. Sustain. Devel., 11(1) (2003) pp. 209–214.

Combined XPS and *ex situ* STM study of the specially prepared model supported silver catalysts was performed. The drastic difference in the Ag particle shape, size distribution and spreading over the support surface were observed for alumina support as compared with pyrographite one. This effect emphasizes the important influence of the substrate nature on the morphology and surface mobility of the supported metal particles.

ELECTRONIC STATE OF COBALT AND OXYGEN IONS IN STOICHIOMETRIC AND NONSTOICHIOMETRIC $Li_{1+x}CoO_2$ BEFORE AND AFTER DELITHIATION ACCORDING TO XPS AND DRS

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J. Power Sources, 119-121 (2003) pp. 669–673.

X-Ray, IRS, XPS, EDRS and magnetic measurements were used to study $Li_{1+x}CoO_2$ ($0 < x \leq 0.1$) samples prepared by conventional ceramic method. It was shown that nonstoichiometric $Li_{1+x}CoO_2$ are characterized by homogeneous crystal structure with statistically distributed vacancies in the cobalt and oxygen layers and the increased Co-O bond covalency. The excess lithium results not in the reduction of Co^{3+} ions, but in the appearance of a new state of oxygen ions different from cell oxide, with higher value of binding energy (BE), i.e. with smaller electronic density. Acid treatment of $Li_{1+x}CoO_2$ leads to the appearance of delocalized (itinerant) electrons. The electronic state of cobalt ions does not change noticeably whereas the additional oxygen state increases significantly, thus, evidencing that oxygen ions do compensate for the charge upon chemical delithiation. The structure of nonstoichiometric samples appeared to be more stable upon this process.

THE INFLUENCE OF NONSTOICHIOMETRY ON THE ELECTRONIC STRUCTURE OF $Li_{1+x}CoO_2$ ($0 < x \leq 0.1$) SUPERSTOICHIOMETRIC OXIDES

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Russ. J. Phys. Chem.,
77(8) (2003) pp. 1319–1323.

$Li_{1+x}CoO_2$ ($0 \leq x \leq 0.1$) samples prepared by the traditional ceramic technique were studied by X-Ray diffraction, IR spectroscopy, X-Ray photoelectron spectroscopy, diffuse reflectance electron spectroscopy, and magnetic measurements. The superstoichiometric oxides had a uniform crystal structure with statistically distributed vacancies in cobalt layers and an enhanced covalence of Co–O bonds. Excess lithium caused the appearance of a new oxygen state (O^-) different from the oxide state (O^{2-}) rather than the reduction of Co^{3+} ions to Co^{2+}. The appearance of oxygen ions with an unusually low electron density was directly related to the formation of oxygen positions with a decreased coordination number; the magnetic properties of $Li_{1+x}CoO_2$ were governed by exchange-coupled (Co^{3+}-O^-) pairs.

THE INFLUENCE OF NONSTOICHIOMETRY ON CHANGES IN THE ELECTRONIC STRUCTURE OF LITHIUM COBALTITE CAUSED BY CHEMICAL DEINTERCALATION OF $Li_{1+x}CoO_2$ ($0 \leq x \leq 0.1$)

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Russ. J. Phys. Chem.,
77(8) (2003) pp. 1445–1451.

Changes in the electronic structure of lithium cobaltites $Li_{1+x}CoO_2$ ($0 \leq x \leq 0.1$) during chemical deintercalation were studied by X-Ray diffraction; IR, X-Ray photoelectron, and diffuse reflectance electron spectroscopy; and magnetic measurements. Acid treatment was shown to cause the partial removal of lithium from the oxide structure and the appearance of delocalized electrons in the system. The electronic state of cobalt ions did not change significantly, whereas oxygen ions were oxidized ($O^{2-} \rightarrow O^{-}$). Structural defects in delithiated oxides had the same nature as in the initial superstoichiometric oxides; these structural defects were low-coordinate oxygen ions in the O^{-} state. The structure of oxides containing excess lithium was stable during chemical deintercalation. The magnetic properties of delithiated oxides were determined by (Co^{3}–O^{-}) exchange-coupled pairs.

FIRST TRIGONAL-ANTIPRISMATIC TRIS-DICHLOROGLYOXIMATE IRON(II) CLATHROCHELATE AND ITS REACTIVITY IN NUCLEOPHILIC SUBSTITUTION REACTIONS

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New J. Chem., 27(7) (2003) pp. 1148–1155.

Tris-dichloroglyoximate clathrochelate $[Fe(Cl_2Gm)_3(SnCl_3)_2]^{2-}$ dianion has been synthesized by a procedure differing from those described earlier for boron-capped analogs. The co-ordinately saturated $SnCl_6^{2-}$ dianion is now used as the capping agent instead of boron-containing Lewis acids. The tris-dichloroglyoximate tin-capped product obtained is far less reactive than its boron-capped analogs, and only in the case of a thiophenolate anion was the regular hexafunctionalized clathrochelate obtained. The complexes synthesized have been characterized by elemental analysis, PD and MALDI-TOF mass, IR, UV-VIS and ^{1}H, ^{13}C and ^{119}Sn NMR spectra, cyclic voltammetry, and X-Ray crystallography for the clathrochelate $[Fe(Cl_2Gm)_3(SnCl_3)_2]^{2-}$ dianion. The geometry of the functionalized complex (the distortion angle φ and main bond lengths in the clathrochelate framework) has been deduced from the quadrupole splitting value in the ^{57}Fe Messbauer spectrum and EXAFS data, respectively.

ESR STUDY OF NANOCRYSTALLINE AEROGEL-PREPARED MAGNESIUM OXIDE

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Phys. Chem. Chem. Phys.,
5(19) (2003) pp. 4299–4305.

Two signals have been observed in the ESR spectra of nanocrystalline MgO synthesized by an aerogel technique. These signals have been assigned to F^{+} centers in the nanocrystals and $–O–{}^{*}CH_2$ radicals formed from residual methoxide groups present at the points of contact between the nanocrystals. The signal of F^{+} centers was found to be thermally stable up to 500°C in oxidizing atmosphere. The second signal was somewhat less stable, and could be removed upon heating to 300°C in the presence of oxygen. Similar organic radicals could be generated by UV irradiation of aerogel prepared (AP) samples, while their concentration appeared to follow the concentration of residual organics in the materials. Irradiation of the samples in the presence of oxygen resulted in the formation of 4-coordinated surface $[O^{-*}O_2]$ radical anions, while no signal typical for 3-coordinated radical anions was observed. Strong Lewis acid and basic sites on the surface of AP-MgO were characterized using the adsorption of 2,2,6,6-tetramethyl-4-oxo-1-oxyl-pyperidine (TEMPONE) and dinitrobenzene, respectively.

SYNTHESIS AND STRUCTURE OF ALKALI-METAL HEXAHYDROPEROXOSTANNATES

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Russ. J. Inorg. Chem., 48(1) (2003) pp. 16–25.

A principal approach to the synthesis of alkali-metal hexahydroperoxostannates $M_2Sn(OOH)_6$ (M = Na, K, Rb) is described. The structure of the resulting hydroperoxo complexes, as determined by IR spectroscopy, NMR (^{119}Sn, ^{2}H, ^{23}Na, ^{87}Rb), EXAFS, and X-Ray powder and single-crystal diffraction, is discussed.

PROTON MOBILITY IN THE COMPOSITES OF IRON ACID SULFATE MONOHYDRATE WITH SILICA

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Mendeleev Commun., 12(6) (2002) p. 223.

The protonic conductivity of the (1–x)$H_3OFe(SO_4)_2 \cdot xSiO_2$ ($x = 0.1–0.6$) composites increased by 1.5–2.0 orders of magnitude and reached its maximal value at $x = 0.3$ for the samples calcined at 380 and 440 K.

EXAFS STUDY OF THE STRUCTURE OF BORATE-GERMANATE GLASSES BASED ON AN $La_3Gd_{10}Eu(BO_3)_6(GeO_4)_2O_8$ SOLID SOLUTION

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Crystallogr. Rep., 48(3) (2003) pp. 355–358.

The nearest environment of europium atoms in borate–germanate glass of composition $La_3Gd_{10}Eu(BO_3)_6(GeO_4)_2O_8$ was studied by EXAFS spectroscopy, and the Eu–O distances were determined. The structural data on the isostructural compound $Gd_{14}(BO_3)_6(GeO_4)_2O_8$ of similar composition were used for the construction of models. It was established that a europium atom is surrounded by eight oxygen atoms, and the Eu–O distance in the glass was equal to ~2.45 Å. These characteristics are close to the values in the crystals of the corresponding solid solutions.

STRIPES AND SUPERCONDUCTIVITY IN THE HTSC COPPER OXIDES

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Physica C, 388-389 (2003) pp. 215–216.

Powder diffraction using synchrotron radiation and high-pressure cell has been performed for the HTSC compound $Hg_{0.8}Tl_{0.2}Ba_2Ca_2Cu_3O_{8.15}$ in the temperature range 100–300 K and external pressure 0–35 GPa. Observed structural anomalies at T_2~240 K and T_1~160 K have been attributed with stripe domain structure. A negative thermal expansion coefficient in a wide temperature range was observed at $P = 1$ GPa. Analysis of crystal structure shows a suppression of T_1 and T_2 features by pressure. As external pressure leads to increase of T_c for investigated material, it was supposed that superconductivity and stripe structure may have the same origin, but their interactions are competing. EXAFS (CuK-edge) measurements support this conclusion.

PHASE SEPARATION IN HIGH-T_C SUPERCONDUCTORS, COPPER OXIDES, AND RELATED ANTIFERROMAGNETIC PHASES CuO And Y_2BaCuO_5

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Crystallogr. Rep., 47(6) (2002) pp. 934–938.

The acoustic properties and crystal structure of high-T_c superconducting cuprates and the related antiferromagnetic phases CuO and Y_2BaCuO_5 exhibit similar properties at a temperature of about 160 K and 240 K. These properties can be associated with the formation of inhomogeneous state of phase separation. Analysis of the magnetic properties of Y_2BaCuO_5 shows that these effects are of a nonmagnetic nature. The results of EXAFS data for the high-T_c superconducting compound $Hg_{0.8}Tl_{0.2}Ba_2Ca_2Cu_3O_{8.10}$ show that the phenomenon of phase separation is suppressed by superconductivity.

STRUCTURE OF THE LIGAND AND SOLVATION SHELLS OF THE GIANT $Pd_{561}PHEN_{60}(OAc)_{180}$ CLUSTER

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J. Struct. Chem.,
44(3) (2003) pp. 376–380.

In an IR spectroscopic study, it have been investigated the ligand and solvation shells of the giant $Pd_{561}Phen_{60}(OAc)_{180}$ cluster, where

Phen = 1,10-phenanthroline and OAc^- are acetate anions, in the solid state and in colloid solutions of acetic acid. Based on the data obtained, the previous idealized model of the cluster which concerns the palladium nucleus-liquid interface was revised. In the solid, the ligand shell of the cluster consists of coordinated Phen and OAc^- ligands with a very low content of noncoordinated outer-spheric acetate anions. In acetic acid colloid solutions, interaction of HOAc molecules with coordinated OAc^- anions results in quantitative removal of the latter from the ligand shell, forming $(OAc \times nHOAc)^- \times kHOAc$ complex anions with n 8 or 9 and k 20. The anions comprise the outer-spheric solvation shell of the cluster, while the coordination shell contains only phenanthroline ligands.

MOLECULAR STRUCTURE OF THE SOLVATED PROTON IN ISOLATED SALTS. SHORT, STRONG, LOW BARRIER (SSLB) H-BONDS

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J. Am. Chem. Soc., 124(46) (2002) pp. 13869–13876.

Large, inert, weakly-basic carborane anions of the icosahedral type $CHB_{11}R_5X_6^-$ (R = H, Me, Cl, Br; X = Cl, Br) allow ready isolation and structural characterization of discrete salts of the solvated proton, $[H(solvent)_x][CHB_{11}R_5X_6]$, (solvent = common O-atom donor). These oxonium ion Brønsted acids are convenient reagents for the tuned delivery of protons to organic solvents with a specified number of donor solvent molecules and with acidities leveled to those of the chosen donor solvent. They have greater thermal stability than the popular $[H(OEt_2)_2][BAr^F]$ acids based on fluorinated tetraphenylborates counterions because carborane anions can sustain much higher levels of acidity. When organic O-atom donors such as diethylether, tetrahydrofuran, benzophenone and nitrobenzene are involved, the coordination number of the proton (x) in $[H(solvent)_x]^+$ is two. A mixed species involving the $[H(H_2O)(diethylether)]^+$ ion has also been isolated. These solid-state structures provide expectations for the predominant molecular structures of solvated protons in solution and take into account that water is an inevitable impurity in organic solvents. The O···O distances are all short, lying within the range 2.36–2.47 Å. They are consistent with strong, linear O···H···O hydrogen bonding. Density functional theory calculations indicate that all $H(solvent)_2^+$ cations have low barriers to movement of the proton within an interval along the O···H···O trajectory, i.e. they are examples of so-called SSLB H-bonds (short, strong, low-barrier). Unusually broadened IR bands, diagnostic of SSLB H-bonds, are observed in these $H(solvent)_2^+$ cations.

ISOLATING BENZENIUM ION SALTS

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J. Am. Chem. Soc., 125(7) (2003) pp. 1796–1804.

When partnered with carborane anions, arenium ions are remarkably stable. Previously investigated only at subambient temperatures in highly superacidic media, protonated benzene is readily isolated as a crystalline salt, thermally stable to >150 ºC. Salts of the type [H(arene)][carborane] have been prepared by protonating benzene, toluene, *m*-xylene, mesitylene and hexamethylbenzene with the carborane superacid $H(CB_{11}HR_5X_6)$ (R = H, Me; X = Cl, Br). They have been characterized by elemental analysis, X-Ray crystallography, NMR and IR methods. Solid state ^{13}C NMR spectra are similar to those observed earlier in solution indicating that lattice interactions are comparable to solution solvation effects. The acidic proton(s) of the arenium cations interact weakly with the halide substituents of the anion via ion-pairing. This is reflected in the dependence of the C-H stretching frequency on the basicity of the carborane anion. Bond lengths in the arenium ions are consistent with predominant *cyclo*-hexadienyl cation character but charge distribution within the cation is less well represented by this resonance form. Structural and vibrational comparison to theory is made for the benzenium ion ($C_6H_7^+$) using DFT at B3LYP/6-31G* and B3P86/6-311+G(d,p) levels. The stability of these salts elevates arenium ions from the status of transients (Wheland intermediates) to reagents. They have been used to bracket the solution phase basicity of C_{60} between that of mesitylene and xylene.

EXTRACTION OF INDIUM FROM SULFURIC ACID SOLUTIONS BY MIXTURES OF DI(2-ETHYLHEXYL)PHOSPHORIC AND OCTANOIC ACIDS

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Solvent Extr. Ion Exch., 20(6) (2002) pp. 765–776.

The extraction of indium from sulfuric acidic solutions by mixtures of di(2-ethylhexyl)phosphoric (D2EHPA, HR) and octanoic (HA) acids was studied. The state of D2EHPA in octanoic acid was investigated by IR-spectroscopy. It was shown that the nonideal behavior in this system occurs due to the partial dimerization of D2EHPA in organic phase. A strong antagonistic effect observed during the extraction of indium is caused by a HR–HA interaction at the expense of formation of intermolecular hydrogen bonds. Low indium concentrations and high excess of extracting agent, as well as application of “inert” diluents, result in the formation of $In(HR_2)_3$ compound in organic phase.

COMPLEXATION OF CARBAMOYLPHOSPHINE OXIDE WITH NITRIC AND PERCHLORIC ACIDS IN WATER-DICHLOROETHANE EQUILIBRIUM SOLUTIONS

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J. Struct. Chem., 44(3) (2003) pp. 365–375.

An IR spectroscopic study has established that in water-dichloroethane equilibrium solutions, carbamoylphosphine oxide forms only one complex with HNO_3, $RR_2P = OHNO_3$, whereas with $HClO_4$ it forms a number of solvation-separated ion pairs (IP). The structure and composition of the cation moiety of these IP depends on the molar ratio C_{CMPO}/C_{HClO4} and the solution preparation temperature. A $CMPO : HClO_4 = 2:1$ complex is formed when $C_{CMPO}/C_{HClO4} > 2$; for $C_{CMPO}/C_{HClO4} < 2$, 1:1 and 1:2 complexes and a complex with $HClO_4$ attached to the tertiary nitrogen of CMPO are formed. A detailed discussion is given for all complexes. It is shown for the first time that H^+ can interact with three oxygen atoms of two $P = O$ groups and one $C = O$ group (or a water molecule) at once. In the absence of CMPO, dichloroethane extracts HNO_3 in the form of micelle-like associates, whose nucleus has a solubilized HNO_3 molecule in the form of a solvation-separated IP.

THE EFFECT OF SiO_2/Al_2O_3 MOLAR RATIO IN MORDENITE UPON THE OPTICAL APPEARANCE OF REDUCED COPPER

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Mater. Sci. Eng., A, 332(1-2) (2002) pp. 174–183.

A series of protonated copper-containing mordenites with variable SiO_2/Al_2O_3 molar ratio (MR) in the range $10 \leq MR \leq 206$ was prepared by ion exchange in copper nitrate aqueous solution. The reduction of copper ions incorporated into the mordenites by hydrogen was shown to lead to different reduced copper species including small metallic particles *inter alia*. The optical appearance of the copper particles depends strongly on the value of MR, however, in a non-monotonic manner in line with the variation of acidity of this series of mordenites. Copper particles formation in the mordenite with MR=15 is almost non-existent, while an efficient reduction proceeds for $MR = 10$ and $20 \leq MR \leq 206$. The optical appearance of copper particles is different and consists of a contribution of the pronounced plasmon resonance maximum at 550–600 nm for $MR = 10$ and $MR = 206$, while for $MR = 20$ and $MR = 31$, it has the shape of shoulder in the same range. These features are simulated using Mie theory, taking into account the size-dependence of the imaginary part of the dielectric constant and the properties of the host medium. The differences in size and particle localization are considered as the main reasons for the difference of the optical features in the visible range.

SULFURIZATION OF POLYMERS.
5. POLY(6-METHYL-5-SULFANYLTHIENO[2,3-B] PYRIDINE-4-THIONE), POLY(THIENO[2,3-B] AZEPINE-4,5(6H)-DITHIONE), AND RELATED STRUCTURES FROM POLY(2-METHYL-5-VINYLPYRIDINE) AND ELEMENTAL SULFUR

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Russ. Chem. Bull., 51(2) (2002) pp. 282–289.

Poly(2-methyl-5-vinylpyridine) is sulfurized with elemental sulfur at 140-320 °C to release hydrogen sulfide and to give black lustrous powders (sulfur content up to 45 %) possessing electric conductivity ($6.4\cdot10^{-11}$ – $1.6\cdot10^{-7}$ S cm^{-1}), paramagnetism (spin concentration $6.2\cdot10^{18}$ – $5.0\cdot10^{19}$ sp g^{-1}, $g = 2.0043$–2.0046, ΔH = 0.49-0.58 mT), and redox and complex-forming properties. Elemental analysis data, IR, ESR, and mass spectra, DSC and TGA data, electric conductivity, electrochemical activity and chemical properties (salt formation and complexation) of the materials synthesized correspond to cross-liked poly(6-methyl-5-sulfanylthieno[2,3-*b*]pyridine-4-thione), poly(thieno[2,3-*b*]azepine-4,5(6*H*)-dithione), and related structures.

SURFACE HETEROGENEITY OF CARBON-SILICA ADSORBENTS STUDIED ON THE BASIS OF THE COMPLEX ADSORPTION INVESTIGATIONS

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Colloids Surf., A, 213(1) (2003) pp. 45–57.

Silica-gel (SG) Si-60 was coated by pyrolytic coke using CVD from methylene chloride. The porous structure of carbon–silica adsorbents (carbosils) was analyzed on the basis of nitrogen adsorption isotherms at 77 K. It has been shown that carbosils are mesoporous adsorbents with complete absence of micropores. Total pore volume and surface area decrease during the carbon deposition on silica surface. Heterogeneity of surface of carbosil samples was estimated by adsorption energy distribution (AEDs) calculated from adsorption isotherms of nitrogen at 77 K and hexane, cyclohexane, benzene and chloroform adsorption isotherms at 473 and 483 K. AEDs were obtained by solving Adsorption Integral Equation with Hill-de Boer kernel function. N_2 AEDs show that distribution of silica active surface sites responsible for N_2 adsorption at 77 K is not altered during the carbon deposition. However, coke deposition leads to improving of polar–apolar surface composition, resulting in increase of adsorption of apolar (hexane) and decrease of adsorption of polar (chlorophorm) substances. The main changes observed in AEDs are connected with decreasing of silica accessible area at stable carbon structure during CVD of carbon.

NEW X-RAY POWDER DIFFRACTION DATA ON δ-Al$_2$O$_3$

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Powder Diffr., 18(4) *(*2003) pp. 309–311.

X-Ray powder diffraction data, high resolution electron microscopy observation and refined unit cell parameters for δ-Al_2O_3 prepared from γ-Al_2O_3 are reported here. The new lattice parameters were $a = 7.9631(7)$, and $c = 23.3975(23)$ Å with space group $P4_12_12$ (No. 92). The new data provide evidence for the simple tripling of the unit cell of the starting γ-Al_2O_3 spinel.

STRUCTURAL STUDY OF TITANIUM DOPED VANADIA AND VANADIUM DOPED TITANIA CATALYSTS

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React. Kinet. Catal. Lett.,
80(1) (2003) pp. 161–169.

The morphologies and structures of nanostructurally assembled V_2O_5 doped with Ti as well as of the inverse system, V-doped TiO_2, have been studied using transmission electron microscopy and Raman spectroscopy. The bulk structure of the Ti-doped vanadia particles was found to be crystallized in a rod-like shape and to have the phase composition of V_2O_5 with titanium atoms nonuniformly distributed over the surface. A coherent interface between supported V_2O_5 and TiO_2 particles was found to be the main structural peculiarity of the inverse system, V-doped TiO_2 (anatase). The vanadium atoms are partially exchanged for titanium atoms at the interface, which leads to a change in the bond lengths of V = O and V-O-Ti in comparison with those observed in the monolayer supported vanadia catalysts. Both materials showed good catalytic behavior in the reaction of selective reduction of NO by NH_3.

SYNTHESIS AND CHARACTERIZATION OF THE TITANIUM DOPED NANOSTRUCTURAL V_2O_5

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Mater. Sci. Eng., A, 343(1-2) (2003) pp. 8–12.

Using scanning and analytical transmission electron microscopies (TEM), the morphology and structure of nanostructurally assembled V_2O_5 doped with Ti has been studied. It was found that the bulk structure of the oxide particles crystallized in rod-like shape is of the V_2O_5 type whereas Ti atoms are located mainly on the thin surface layer of the rods. Such surface coating is nonuniform and contains up to 3 at. % of titanium. Modification of the oxide sample with titanium atoms seems to stabilize the V_2O_5 structure against electron beam irradiation.

STRUCTURE INVESTIGATION OF SUBSURFACE LAYER OF PLATINAZED GOLD BY THE METHOD OF X-RAY GRAZING INCIDENCE

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Surf. Invest.: X-Ray, Synchr. Neutron Techn., 11 (2003) pp. 48–51.

The surface investigation of Pt/Au subsurface layers was carried out by the method of X-Ray grazing incidence on the station of precision powder diffractometry Siberian Synchrotron Radiation Center (Budker Institute of Nuclear Physics, Novosibirsk). The dependence of 111 and 200 Au and Pt reflection positions on the angle of radiation beam incidence in the range of 5^o-1^o was studied. It is shown that at electrolytic deposition of Pt onto polycrystalline Au substrate the intermediate layer of substitution solid solution is formed on the Pt-Au interface.

STRUCTURE CHARACTERISTICS OF DISORDERED ZIRCONIUM HYDROXOXIDES

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Crystallogr. Rep., 48(3) (2002) pp. 413–415.

The structural characteristics of low-temperature zirconium hydroxoxide and zirconium dioxide obtained from zirconyl nitrate and treated at 383 and 653 K have been studied by the X-Ray method of distribution of radial electron density. It is shown that the low-temperature hydroxide contains a ~ 10 to 15 Å nucleus of the crystalline phase with a structure of short-range order similar to the short-range order in ZrO_2. An increase in treatment temperature of zirconium hydroxide results in the formation of a mixture of cubic and monoclinic zirconium dioxide with a particle size of ~ 60 Å.

STRUCTURAL PECULIARITIES OF ANOMALOUS ELECTROLYTIC PALLADIUM DEPOSITS PREPARED UNDER HYDRIDE FORMATION CONDITIONS

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Russ. J. Electrochem., 39(3) (2003) pp. 253–262.

The peculiarities of bulk and surface structures of electrolytic palladium deposits formed under hydride formation conditions are studied by X-Ray diffraction (XRD) and X-Ray photoelectron spectroscopy techniques. For anomalous deposits with high hydrogen capacities, the evolution of the XRD behavior is traced as a function of thermal treatment. The material is shown to comprise two cubic phases with different lattice parameters.

FACE-CENTERED CUBIC AND HEXAGONAL CLOSED-PACKED NANOCRYSTAL SUPERLATTICES OF GOLD NANOPARTICLES PREPARED BY DIFFERENT METHODS

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J. Phys. Chem. B, 107(30) (2003) pp. 7441–7448.

Dodecanethiol-stabilized gold nanoparticles with similar average size organize into different superlattice structures depending upon the method of preparation of the nanocrystals. Particle synthesized by the inverse micelle technique preferentially assemble into face-centered cubic (fcc) structures with long-range translational and orientational ordering. Gold nanoparticles obtained by the solvated metal atom dispersion (SMAD) method behave like "hard" spheres and predominantly organize into hexagonal close-packed (hcp) nanocrystal superlattices with long-range translational ordering. Different packing behavior results from differences in nanoparticle core morphologies induced by the synthetic method; fcc ordering is preferred by single crystalline nanoparticles, while hcp is preferred by polycrystalline nanoparticles. A combination of optical microscopy, transmission electron microscopy (TEM and HRTEM), selected area electron diffractions (SAED), atomic force microscopy (AFM) and X-Ray diffraction (XRD) were used to characterize both the dispersed nanoparticles and the nanocrystal superlattices.

HIGH SURFACE AREA HOMOGENEOUS NANOCRYSTALLINE BIMETALLIC OXIDES OBTAINED BY HYDROLYSIS OF BIMETALLIC μ-OXO ALKOXIDES

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J. Mater. Chem., 13(2) (2003) pp. 410–414.

Homogeneously dispersed bimetallic oxides in nanocrystalline or amorphous forms, of the type MAl_2O_4 (where M = Mg, Ca, Mn, Co, Fe, and Zn) were prepared from bimetallic oxo-bridged alkoxides $[(RO)_2Al–O–M–O–Al(OR)_2]$, where the Al–O–M–O–Al bonds were not hydrolytically cleaved. This approach yields hydroxides $[(HO)_2Al–O–M–O–Al(OH)_2]$ which, upon thermal dehydration, yield oxides [OAl–O–M–O–AlO], such that M is homogeneously dispersed with an empirical formula of MAl_2O_4. These materials were obtained in high surface area forms and were characterized by X-Ray diffraction, electron microscopy, surface area analyses, and solid-state ^{27}Al NMR. Comparative studies of the hydrolysis of alkoxo-bridged alkoxides yielded mixed metal oxide phases with lower surface areas.

UNUSUAL BEHAVIOR OF NANOCRYSTALLINE STRONTIUM OXIDE TOWARD HYDROGEN SULFIDE

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J. Nanopart. Res., 4(4) (2002) pp. 357–366.

The thermodynamically favored reaction of solid strontium oxide with gaseous hydrogen sulfide is kinetically enhanced to a large degree by the use of higher surface area nanocrystalline SrO in the form of brush-like collections of metal oxide fibers. An unusual feature is that the reaction $SrO + H_2S \rightarrow SrS + H_2O$ proceeds stoichiometrically at room temperature, but at higher temperatures the reaction efficiency goes down, apparently due to rapid temperature induced crystal growth of the nanocrystalline SrO. The samples studied vary in crystallite size from 20 to 27 nm, while average particle size (nanocrystal aggregates) corresponds to aerogels SrO sizes (~100 nm).

OXOVANADIUM(V) CHLORIDE COMPLEXES

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Russ. J. Inorg. Chem., 47(12) (2002) pp. 1860–1863.

Electronic absorption and IR spectroscopy and ^{51}V NMR showed that dimeric chloride complexes $[V_2O_3(H_2O)_{8-n}Cl_n]^{(4n)+}$ are formed in the V(V)–HCl–LiCl–H_2O system at the ionic strength $I = 11.0$ mol/l, 0 °C, $C_{HCl} \leq 0.1$ mol/l, and $C_V > 0.015$ mol/l. At high concentrations of hydrochloric acid, in the vanadium(V) concentration range $2 \times 10^{-4} – 3 \times 10^{-2}$ mol/l only mononuclear complexes of the H_nVOCl_{3+n} (n = 0–1) type exist.

NITROXYL RADICALS AS SPIN PROBES FOR THE STUDY OF LEWIS AND BRONSTED ACID SITES OF OXIDE CATALYSTS

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"Magnetic Resonance in Colloid and Interface Science",
Eds. J. Fraissard and O. Lapina, NATO ASI Series,
Kluwer Academic Publishers, The Netherlands, 2002,
pp. 625–630.

An opportunity of use in common of iminoxyl and imidazoline radicals for detection of Lewis and Bronsted acid sites on the surface of γ-Al_2O_3 as well as for the study of their properties is shown.

FEATURES OF THERMAL DEGRADATION OF POROUS POLYMETHACRYLATE NANOCOMPOSITES

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Polym. Sci., A, 45(6) (2003) pp. 560–563.

The thermal degradation of porous polymethacrylates filled with silver nanoparticles and the morphology of their degradation products were investigated by thermoanalysis and scanning electron microscopy. It was shown that the photoreduction of silver nanoparticles *in situ* results in a decrease in the thermal stability of nanocomposites. The size of silver aggregates resulting from the degradation process was found to be dependent on the parameters of the porous structure of the material used. A mechanism describing the formation of silver mesostructures upon degradation of the porous nanocomposites was proposed.

FEATURES OF PHASE FORMATION IN MIXED ZnS-EuS THIN FILMS GROWN BY METALORGANIC CHEMICAL VAPOR DEPOSITION

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Mater. Res. Bull., 38(3) (2003) pp. 409–420.

The phase composition of the mixed ZnS–EuS films deposited from volatile dithiocarbamates has been studied using differential dissolution technique (chemical method of the phase analysis) and electron microscopy. Phase composition was found to depend on the Eu content in the films, that in turn depends on a flow density ratio of the Eu and Zn volatile precursors. A single-phase solid solution, $Zn_{0.998}Eu_{\leq 0.002}S$, was observed only for films with Eu content ≤ 1 mol %, other films were found to be two-phase. For films with the Eu content between 2 and 16 % and above 80 %, impurity phases, EuS and ZnS, respectively, were detected by differential dissolution technique. They evolved as low-sized sulfide precipitates encapsulated in an organic coat. No impurity phases in the films of the same Eu content were noticed by X-Ray technique and Raman spectroscopy. For the films with the Eu content between 16 and 80 %, sulfide phases, ZnS and EuS, were found to be free from any organic coat, and structural methods as with differential dissolution technique were also capable of observing the phases. Conditions are given to prepare Eu doped ZnS films of good quality by MOCVD technique.

THERMODYNAMIC AND ADSORPTION PROPERTIES OF SEMIINTERPENETRATING POLYMER NETWORKS BASED ON POLYBENZIMIDAZOLES AND POLYAMINOIMIDE RESIN

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Russ. Chem. Bull., 52(5) (2003) pp. 1083–1093.

Thermodynamic characteristics of adsorption of organic compounds on semiinterpenetrating networks based on polybenzimidazoles and polyaminoimide resin with different compositions were studied at small coverages using inverse gas chromatography. The following characteristics were determined: adsorption equilibrium constants (specific retention volumes) of substances of different classes (n-alkanes, aromatic hydrocarbons, ethers, ketones, alcohols, and nitrogen- and halogen-containing compounds), appropriate changes in differential molar internal energy and Helmholtz potential, and changes in standard molar entropy of the sorbates. The contributions of the molecular fragments to the heat of adsorption were calculated. The adsorption properties of the semiinterpenetrating networks based on polybenzimidazoles and polyaminoimide resin differ from those of the starting polymeric materials and their physical mixtures with the similar composition. Unlike graphitized thermal carbon black (nonspecific adsorbent), the network and starting materials manifest the specific properties (electron-donating and electron-accepting). The difference in the thermodynamic characteristics of adsorption on the semiinterpenetrating polymeric networks with different compositions is determined by the size and geometry of interphase regions.

METHODS OF STOICHIOGRAPHY IN GEOCHEMISTRY AND MINERALOGY

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Spectrochim. Acta, Part B, 58(2) (2003) pp. 373–386.

Reported is a novel reference-free technique, based on stoichiography, for the molecular and phase analysis of complex mixtures with unknown compositions. The concept of stoichiography is based on the stoichiometry of mass transfer of the constituents in transient, homogeneous and heterogeneous phase transformation processes. The technique utilizes both the separation of components according to their differential dissolution characteristics as well as the dynamics of the changes in stoichiometry. The detailed study of the dissolution processes has been made possible by the use of a specially designed instrumental system, termed a Stoichiograph, which consists of a high sensitive inductively coupled plasma atomic emission spectrometer as the detector–analyzer. Fundamentals, methodology, and instrumentation of the technique are discussed and its application for the phase analysis of multielement-multiphase samples such as minerals, aerosols, and archaeological materials is demonstrated.

MANIFESTATION OF GRANULAR STRUCTURE IN FMR SPECTRA

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J. Magn. Magn. Mater., 267(1) (2003) pp. 13–18.

The ferromagnetic resonance (FMR) method is used to study ferromagnetic powders dispersed in a diamagnetic solid matrix. The fine structure observed against a background of wide structureless FMR lines, which are common for polycrystalline non-oriented specimens, have been investigated. According to the suggested model, the observed narrow lines appear in FMR spectra owing to jump changes in resonance conditions resulting from abrupt changes of the specimen magnetization with varying the outer magnetic field. It is shown that physical reasons of the magnetization jumps may be the magnetic interparticle interaction as well as the complex anisotropy of particles.

GENERATION OF O_2^- ION-RADICALS IN ZIRCONIUM DIOXIDE UPON MECHANOCHEMICAL ACTIVATION

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Chem. Phys., 22(11) pp. 25–29.

An effect of mechanochemical activation on generation of defects and reactivity of ZrO_2 is studied by ESR method. It is shown that mechanochemical activation of ZrO_2 is accompanied by reduction process resulting in formation of F-centers and ion-radicals O_2^-. An effect of ZrO_2 surface sulfatisation on the stated centers is revealed.

SORPTION AND SENSING CHARACTERISTICS OF POLYVINYL ALCOHOL FILMS IMPREGNATED WITH $CaCl_2$

D.V. Andreev, L.L. Makarshin, V.N. Parmon

React. Kinet. Catal. Lett., 80(1) (2003) pp. 181–188.

PVA-$CaCl_2$ composites were studied as humidity sensors. The composites give a relevant conductivity variation of 4.5–5 orders of magnitude in a wide range of relative humidity (0-86 %). Water sorption isotherms evidence the existence of a size effect in the formation of $CaCl_2 \cdot nH_2O$ crystalline hydrate.

AEROGEL AS CHERENKOV RADIATOR FOR RICH DETECTORS

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Nucl. Instrum. Methods Phys. Res., Sect. A, 502(1) (2003) pp. 227–230.

The results obtained using silica aerogel as Cherenkov radiator for the separation and identification of particles in the momentum range from 6 to 10 GeV/*c* are presented. Photoelectron yield and Cherenkov ring resolution were studied under different experimental conditions.

RECENT RESULTS ON AEROGEL DEVELOPMENT FOR USE IN CHERENKOV COUNTERS

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Nucl. Instrum. Methods Phys. Res., *Sect. A*, 494(1-3) (2002) pp. 491–494.

Synthesis of silica aerogel for Cherenkov counters is being studied for more than 10 years at the Boreskov Institute of Catalysis in collaboration with the Budker Institute of Nuclear Physics. Index of refraction, light scattering length and light absorption length are optical characteristics, which determine the quality of aerogel Cherenkov counter. These parameters were measured for the aerogel produced. The results are presented.

ASHIPH COUNTERS FOR THE KEDR DETECTOR

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Nucl. Instrum. Methods Phys. Res., *Sect. A*, 494(1-3) (2002) pp. 424–429.

The status of the ASHIPH (Aerogel, wavelength SHIfter, and PHotomultipliers) system of the KEDR detector is described. The measurement of the quality of the particle identification with the ASHIPH counters was performed. The π/K separation is 4.5σ for the momentum 1.2 GeV/c and 4.7σ for the momentum 0.86 GeV/c. Timing properties of the ASHIPH counter are measured. The time resolution for pions is 2 ns, and the BBQ decay time is 15 ns. The advantages and disadvantages of Cherenkov counters filled with aerogel crumb are discussed. The process of the mass counter production for the KEDR detector is described.

CHERENKOV RINGS FROM AEROGEL DETECTED BY FOUR LARGE-AREA HYBRID PHOTODIODES

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(*University of Milano-Bicocca and INFN, Milano, Italy; **CERN, Geneva, Switzerland; ***Budker Institute of Nuclear Physics, Novosibirsk, Russia; ****Rutherford Appleton Laboratory, Chilton, UK; *****Imperial College, London, UK; ******University of Cambridge, Cambridge, UK)

Nucl. Instrum. Meth. Phys. Res., *Sect. A*, 504(1-3) (2003) pp. 290–293.

The results obtained using thick samples of silica aerogel as radiators for a Ring Imaging Cherenkov counter are reported. Four large-diameter hybrid photodiodes with 2048 channels have been used as photon detectors. Pions and protons with momenta ranging from 6 to 10 GeV/*c* were separated and identified. The number of photoelectrons and the radius of the Cherenkov rings together with the Cherenkov angle resolution were measured. A comparison with a simulation program based on GEANT4 is discussed.

DEVELOPMENT OF THRESHOLD AEROGEL CHERENKOV COUNTERS ASHIPH FOR THE SND DETECTOR

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(*Budker Institute of Nuclear Physics, Novosibirsk, Russia)

Nucl. Instrum. Methods Phys. Res., Sect. A, 494(1-3) (2002) pp. 487–490.

The paper is devoted to the development of Cherenkov counters based on the Aerogel, wavelength SHIfters and PHotomultiplier tubes (ASHIPH) for the SND detector at VEPP-2000. The ASHIPH counter system for the SND detector is designed. The counters will separate π and K mesons in the momentum range from 300 to 900 MeV/*c*. Optical properties of aerogel samples with refraction index 1.13 are measured and results are presented. As photodetectors, the microchannel plate photomultipliers with multialkali photocathodes are used. Monte Carlo simulation of the ASHIPH counter predicts more than 7 photoelectrons for a relativistic particle.

PHASE AND ELEMENTAL COMPOSITION AND DISTRIBUTION OF URINARY CALCULI IN PATIENTS FROM NOVOSIBIRSK AND OMSK REGIONS

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T.N. Grigorieva, A.I. Nizovskii,**
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Chem. Sustain. Devel,
11(4) (2003) pp. 581–587.

Investigation of endemic features of urolithiasis taking into account local factors, both natural and technology-related ones, allows one to obtain additional information about one of the reasons of this disease. Mineral composition and distribution of urinary calculi in patients from Novosibirsk and Omsk Regions are investigated. A common feature of urolithiasis in the regions under comparison is noticeable predominance of oxalate urinary calculi. However, at the conservation of the general trend of distribution with respect to the prevailing component, patients from Novosibirsk Region exhibit an increase in phosphate and decrease in urate urolithiasis. Noticeable differences in paragenesis of minerals comprising multicomponent urinary calculi and in the composition of single-component concretions are observed. In the Novosibirsk samples, single-mineral concretions are more frequently composed of whwellite, while in the Omsk samples it is anhydrous uric acid. Comparative analysis of the mineral composition and distribution of urinary calculi in other regions according to literature data was carried out.

Fundamental and Practical Approaches to Catalyst Preparation

SYNTHESIS OF HETEROPOLY ACIDS AND THEIR SALTS USING MECHANOCHEMICAL ACTIVATION

V.V. Molchanov, G.M. Maksimov,
R.I. Maksimovskaya, V.V. Goidin, R.A. Buyanov

Inorg. Mater., 39(7) (2003) pp. 687–693.

A method is proposed for the synthesis of heteropoly acids from oxides of molybdenum, tungsten, and vanadium via mechanochemical activation. The fundamental principles of this approach to the synthesis of heteropoly acids containing different ligands and heteroatoms are formulated. The new $V_2O_5{\cdot}nMoO_3$ compounds synthesized in this work are found to be highly reactive with phosphoric acid, which is due to the unsaturated coordination of the vanadium cations and the low structural perfection of these compounds. The application area of the proposed method is established. It appears to be most effective in the synthesis of phosphomolybdovanadic and phosphomolybdic heteropoly acids. In some instances, heteropoly acids can be prepared by solid-state reactions, which makes it possible to use $V_2O_5{\cdot}nMoO_3$ compounds with $n \leq 6$ as starting reagents. The method has a number of important advantages: the process is waste-free, requires a shorter synthesis time and involves a smaller number of steps as compared to the existing processes, affords an increased yield of heteropoly acids, and involves no explosion- or fire-hazardous steps.

EFFECT OF MECHANOCHEMICAL ACTIVATION ON THE CATALYTIC PROPERTIES OF FERRITES WITH THE SPINEL STRUCTURE

V.V. Molchanov, R.A. Buyanov,
Yu.T. Pavlyukhin* (*Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia)

Kinet. Catal., 44(6) (2003) pp. 788–792.

It was found experimentally that stacking defects formed in the mechanochemical activation of zinc ferrite enhanced the specific catalytic activity in the reaction of CO oxidation. The specific rate of CO oxidation was a linear function of defect concentration, which was determined using Mössbauer spectroscopy and X-Ray diffraction. A conclusion was drawn that the same centers are responsible for an increase in the catalytic activity, the sorption capacity for hydrogen sulfide, and the reactivity of zinc ferrite in the interaction with hydrochloric acid. It was assumed that analogous factors caused an increase in the catalytic activity and reactivity of magnesium ferrite.

NATURE AND REGULARITIES OF THE EFFECT OF MECHANOCHEMICAL ACTIVATION ON CATALYTIC ACTIVITY

R.A. Buyanov, V.V. Molchanov

Chem. Sustain. Devel., 11(3) (2003) pp. 467–470.

Changes in thermodynamic and kinetic characteristics of catalytic processes under mechanochemical activation of catalysts (mechanochemical catalysis) are considered. It is shown that the activity of catalysts should increase under the mechanochemical activation, while selectivity can vary depending on the relations between the changes in the target reaction and side processes. The considered phenomena are formulated as a new research area, which is at the very beginning of its development.

PHYSICO-CHEMICAL BASES OF PREPARATION OF MASSIVE OXIDE CATALYSTS FOR DEEP OXIDATION USING MECHANOCHEMICAL ACTIVATION.

1. SPECIFICITY OF USING MECHANOCHEMICAL TECHNIQUE IN PREPARATION OF MASSIVE OXIDE CATALYSTS

L.A. Isupova, V.A. Sadykov

Catal. Ind., 4 (2003) pp. 3–16.

The paper considers application of the mechanical treatment as a stage in synthesis of simple (CuO, Co_3O_4, Fe_2O_3, MnO_x), or mixed oxides with perovskite structure ($La_{1-x}Me^1_xMe^2O_3$, where Me^1 = Sr, Ca, ..., Me^2 = Mn, Co, Ni, Fe) for oxidation processes that is the way for wasteless catalyst's preparation technology elaboration. Effect of mechanical treatment on the catalytic activity and on the catalyst preparation stages is discussed.

For dispersed 3d oxides (CuO, Co_3O_4, Fe_2O_3, MnO_x), their mechanical activation in an air was shown to change the size of particle aggregates, separate crystallites, grain sizes within crystallites and density of point and extended defects. Along with defect structure variation, mechanical activation is accompanied by the surface hydration and carbonization, which is reflected in the catalytic activity decline.

For complex perovskite oxides $La_{1-x}Me^1_xMe^2O_3$, (where Me^1 = Sr, Ca, ..., Me^2 = Mn, Co, Ni, Fe) prepared via the mechanical activation route, specificity of their phase composition and microstructure was elucidated. Catalytic properties of perovskites were reliably proved to depend upon their microstructure determined by the synthesis parameters including mechanical activation and subsequent annealing of the activated mixture of solid reagents at different temperatures.

These fundamental results were applied for development of practical oxidation catalysts comprised of bulk oxide systems, which have passed successfully pilot-industrial tests. Monolith catalysts for ammonia oxidation into nitrogen oxides under pressure are now widely used in practice for the weak nitric acid production instead of a part of the platinum gauzes.

PHYSICO-CHEMICAL BASES FOR PREPARATION OF MASSIVE OXIDE CATALYSTS FOR DEEP OXIDATION USING MECHANOCHEMICAL ACTIVATION.

2. MASSIVE MODULAR OXIDE CATALYSTS FOR HIGH TEMPERATURE OXIDATION PROCESSES

L.A. Isupova, V.A. Sadykov

Catal. Ind., 5 (2003) pp. 3–12.

The paper gives the results of the studies related to using the mechanochemicasl method in preparation of monolith oxide catalysts for high-temperature oxidation processes including those for methane and ammonia oxidizing. The mechanochemical method and equipment for machine work of solids are promising in production of oxide catalysts thus allowing producing complex oxides of high specific surface without their decomposition as well as solving the problems of granule formability and strength improvement. The effect of preparation conditions on properties of oxides has been investigated. Based on the studies carried out, the monolith honeycomb structure catalysts have been developed for high-temperature oxidation processes – IC-12-83, and IC-42-1. A production section was established on the bases of Scientific and Technological Department of Applied Catalysts of the Boreskov Institute of Catalysis to produce honeycomb monolith (as large as 10 m^3/year).

DEVELOPMENT OF Fe_2O_3-BASED CATALYSTS OF DIFFERENT GEOMETRIES FOR ENVIRONMENTAL CATALYSIS

L.A. Isupova, V.A. Sadykov, S.V. Tsybulya, G.S. Litvak, G.N. Kryukova, E.B. Burgina, A.V. Golovin

Chem. Sustain. Devel.,
11(1) (2003) pp. 89–100.

X-Ray, TA, IRS, TEM and BET techniques were used to study the effect of mechanical treatment in a centrifugal planetary ball mill EI 2×150 and in a continuously operating vibration ball mill VCM-25 on physicochemical properties of powdered iron oxide of different prehistory, as well as on the properties of produced granulated supports and catalysts. The influence of structure-forming additives and electrolyte was discussed. The influence of the method used for introduction of the active component on the catalyst properties for complete oxidation of butane and CO was established.

FORMATION OF NANOCRYSTALLINE STRUCTURES IN A Co-Al SYSTEM BY MECHANICAL ALLOYING AND LEACHING

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J. Alloys Compd., 351(1–2) (2003) pp. 101–105.

Phase composition of the materials obtained by mechanical alloying of system Co-Al (Al concentration ranges from 50 to 70 at. %) and removal of aluminum from such alloys was investigated by differential dissolution, X-Ray phase analysis and TEM with a resolution of 0.4 nm. The intensive mechanical alloying provides formation of the nanocomposite material containing both amorphous phase Co_2Al_5 and nanocrystalline particles of phase CoAl. Leaching of amorphous phase Co_2Al_5 result in the amorphous cobalt containing admixtures of alumina and hydroxide. Nanocomposite amorphous phase Co_2Al_5 and CoAl convert into nanocomposite amorphous Co and b.c.c. Co.

POROUS Al_2O_3/Al METAL CERAMICS PREPARED BY THE OXIDATION OF ALUMINUM POWDER UNDER HYDROTHERMAL CONDITIONS FOLLOWED BY THERMAL DEHYDRATION. 3. THE REACTIVITY OF ALUMINUM, THE REACTION MECHANISM OF ITS OXIDATION WITH WATER VAPOR, AND THE MICROTEXTURE OF CERMETS

S.F. Tikhov, Yu.V. Potapova, V.A. Sadykov, V.B. Fenelonov, S.V. Tsybulya, A.N. Salanov, V.P. Ivanov, V.N. Kolomiichuk

Kinet. Catal., 44(2) (2003) pp. 297–308.

The macrokinetics of aluminum oxidation under hydrothermal conditions at 150–250 °C and water vapor pressures of ~0.5–4.5 MPa was studied. The apparent kinetic characteristics of the process were determined. The diffusion of water through the layer of a hydrated product was found to be a rate-limiting step. It was found that diffusion coefficients for various aluminum samples differed by almost two orders of magnitude; the main reaction steps were revealed. Changes in the texture of aluminum oxide in cermets in the course of the hydrothermal oxidation reaction were analyzed. This texture was found to depend on the ratio between the specific rate of the oxidation reaction and the rate of aging of the oxidation products under hydrothermal conditions.

STRUCTURAL ASPECT OF A THERMAL ACTIVATION EFFECT IN THE $MnO_x/\gamma\text{-}Al_2O_3$ SYSTEM

S.V. Tsybulya, G.N. Kryukova, T.A. Kriger, P.G. Tsyrulnikov

Kinet. Catal., 44(2) (2003) pp. 287–296.

Solid-phase reactions in the aluminum–manganese oxide system, including the structural mechanism of the thermal activation of catalysts, were studied at temperatures up to 1100 °C. It was found that the solid-phase reaction at 900–1000 °C occurred via two pathways because of the diffusion of manganese ions to aluminum oxide and aluminum ions to manganese oxide. Nanoheterogeneous state of the active component, which was observed in the range 25–600 °C, is the product of incomplete decomposition of the high-temperature aluminum–manganese phase $Mn_{2.1-x}Al_{0.9+x}O_4$ ($0 \le x \le 0.6$) with a cubic spinel structure; this phase was equilibrium at the synthesis temperature but metastable below 650 °C.

CHARACTERIZATION OF THE NICKEL-AMESITE-CHLORITE-VERMICULITE SYSTEM. 1. SILICON BINDING IN Ni–Mg–Al PHYLLOALUMINOSILICATES

A.A. Khassin, T.M. Yurieva, M.P. Demeshkina, G.N. Kustova, I.Sh. Itenberg, V.V. Kaichev, L.M. Plyasova, V.F. Anufrienko, I.Yu. Molina, T.V. Larina, N.A. Baronskaya, V.N. Parmon

Phys. Chem. Chem. Phys., 5(18) (2003) pp. 4025–4031.

Synthetic TO (1 tetrahedral layer/1 octahedral layer) phylloaluminosilicates of Ni–Mg–Al with amesite (septechlorite) structure were synthesized and their evolution during calcination in inert and reducing media was studied. After treatment at 700–800 °C in hydrogen, the samples consisted of dispersed metallic nickel particles supported on TOT Mg-chlorite-vermiculite; none of the catalysts studied contained SiO_2. The samples were stable in inert gas and hydrogen atmospheres at 850 °C, as well as in hydrogen plus steam at 20 bar and 650 °C. Thus, Ni-containing amesite-like compounds are considered to be suitable catalysts for the methane steam reforming process.

THE SYNTHESIS AND STRUCTURE OF A SINGLE-PHASE, NANOCRYSTALLINE MoVW MIXED-OXIDE CATALYST OF THE Mo_5O_{14} TYPE

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J. Catal., 215(2) (2003) pp. 177–187.

The different preparation steps are characterized for the single-phase, crystalline, ternary oxide $(MoVW)_5O_{14}$, which is important for catalytic, mild selective oxidation reactions. For the synthesis of this oxide, solutions of ammonium heptamolybdate, ammonium metatungstate, and vanadyl oxalate were spray-dried followed by different thermal treatments. The structures of the materials formed at each preparation step, starting from the precursor to the final product, were studied using scanning and transmission electron microscopy, X-Ray powder diffraction, thermal analysis, and Raman spectroscopy. Raman spectroscopy was also applied to shed some light into the aqueous chemistry of the mixed precursor solutions. Raman data indicate that a molecular structure which seems to be closely related to that of the final crystalline Mo_5O_{14}-type oxide is already formed in solution. X-Ray diffraction revealed that the thermal treatment steps strongly affect the degree of crystallinity of the ternary Mo_5O_{14} oxide. Transmission electron microscopy with energy-dispersive microanalysis confirmed the presence of V and W in the molybdenum oxide particles and gave evidence for the (010) plane as the most developed face of the crystals of this phase. Details of the structural transformation of this system at the different preparation and calcination steps are discussed in relation to their performance in the selective partial oxidation of acrolein to acrylic acid.

THE ROLE OF SUPPORT IN FORMATION OF THE MANGANESE–BISMUTH OXIDE CATALYST FOR SYNTHESIS OF NITROUS OXIDE THROUGH OXIDATION OF AMMONIA WITH OXYGEN

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J. Catal., 221(1) (2003) pp. 213–224.

BET, XRD, XPS, and TPR by hydrogen were used for investigation of supported Mn–Bi oxide catalysts for ammonia oxidation into nitrous oxide. The catalysts were synthesized by impregnation of γ-, α-Al_2O_3 and SiO_2 with solutions of manganese and bismuth nitrates. The character of phase transformations, surface concentration, and state of the active component were shown to depend on the nature of the support. The sequence stabilization of active constituents of the Mn–Bi–O/α-Al_2O_3 catalyst and types of the stabilized species were determined. The activity of the Mn–Bi–O supported catalysts calcined at 400 °C was established to equal 95–97 % and to be practically independent of the support nature, while the activity decreased with elevation of the calcination temperature. The Mn–Bi–O/α-Al_2O_3 catalysts exhibited the highest selectivity to N_2O (84.4%) under identical conditions. The correlation between the $Mn^{3+}/Mn^{\delta+}$ $(2 < \delta < 3)$ ratio in the catalyst and the selectivity to N_2O was revealed.

ALKYLATION OF ISOBUTANE WITH BUTENES ON ZIRCONIUM SULFATE CATALYSTS

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Russ. J. Appl. Chem., 76(4) (2003) pp. 550–557.

Sulfated zirconia catalysts supported on silica gel and aluminum oxide were prepared by impregnation, and their structure and acid-base and catalytic properties were studied. The parameters of synthesis and characteristics of this catalyst, which ensure high activity and selectivity in liquid-phase alkylation of isobutane with butenes, were determined.

HIGH-LOADED NICKEL–SILICA CATALYSTS FOR HYDROGENATION, PREPARED BY SOL–GEL ROUTE: STRUCTURE AND CATALYTIC BEHAVIOR

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Appl. Catal. A: General,
245(2) (2003) pp. 277–288.

Ni/SiO_2 catalysts (from 50 to 95 wt. % of nickel) were prepared by the heterophase sol–gel method through impregnation of dispersed hydrated nickel oxide with commercial ethyl silicate-32. Impregnation of a porous metal precursor with alcoholic solution of the ethyl silicate followed by drying makes it condensed to form polysiloxane films directly on the precursor surface. The next steps of calcination and reduction lead to formation of a silica matrix with metal nanoparticles confined in its pores.

^{29}Si NMR, IR spectroscopy, differentiating dissolution, temperature-programmed reaction (TPR), X-Ray powder diffraction (XRD) and transmission electron microscope (TEM) techniques were used for studies of the precursors and catalysts. It was shown that silicate species favoring formation of fine nickel particles under reduction were produced by interaction of hydrated NiO with ethyl silicate. As the silica content increased from 5 to 52 %, the nickel particles decreased in size from 10 to 4 nm. The sol–gel catalysts were tested in the reaction of benzene hydrogenation to show that the nickel surface was not blocked by silica but exposed to reactants. As a result, the observed catalytic activity was higher than the activity of a number of commercial nickel catalysts.

SYNTHESIS OF ULTRADISPERSED NICKEL PARTICLES BY REDUCTION OF HIGH-LOADED NiO-SiO$_2$ SYSTEMS PREPARED BY HETEROPHASE SOL-GEL METHOD

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S.V. Cherepanova, L.M. Plyasova

J. Phys. Chem. B,
106(46) (2002) pp. 11922–11928.

TPR, XRD, TEM, and IR techniques were used for studying reduction of nickel-silica systems over the whole concentration range (nickel content was varied within the range 16 to 95 %). The systems were prepared by the heterophase sol-gel method. It was established that the reduction temperature increased as the silica content increased from 0 to 34 % in the system, the average size of nickel crystallites being decreased from 44 to 4.5 nm. At the further increasing the silica content (to 84 %): the reduction temperature decreased while the nickel crystallites grew in size to 15 nm. Testing of the prepared systems in benzene hydrogenation showed that the surface of nickel particles was accessible to the reactants.

Mo/ZSM-5 CATALYSTS FOR METHANE AROMATIZATION. STUDY OF THE Mo PRECURSOR SPECIES IN IMPREGNATION SOLUTION OF AMMONIUM HEPTAMOLYBDATE

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V.V. Kuznetsov

Chem. Sustain. Devel.,
11(1) (2003) pp. 167–171.

A change in the ratio between monomeric and polymeric molybdenum species regarding the concentration and pH of the impregnation solutions will probably make a significant effect on the nature and number of active sites of Mo/ZSM-5 catalysts. To provide the control of molybdenum species in solutions, dependence of structure of molybdenum species in the initial impregnation solutions of ammonium heptamolybdate on the concentration and pH of these solutions (from electron absorption spectra) has been studied. When the concentration of solutions is low or pH increases, there are no polymeric molybdenum species. Besides, there is a region where monomeric and polymeric species exist at a time. At higher concentrations or when pH decreases, monomeric species transform almost completely into polymeric species.

RELATIONSHIP BETWEEN SURFACE PROPERTIES OF MODIFIED TITANOOXIDES AND THEIR CATALYTIC PERFORMANCE IN THE REACTION OF ETHYLENE GLYCOL ETHOXYLATION

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Chem. Sustain. Devel.,
11(1) (2003) pp. 123–130.

Relationship of structure and surface properties of modified titanium dioxides, prepared by alkoxide method using derivatives of phosphoric acid as precursors, with their catalytic performance in the reaction of ethylene glycol ethoxylation was investigated. It was found that such catalysts are mono-phase, nanocluster ones with anatase structure, and have uniform narrow pore distribution. Catalysts prepared using the amidophosphite precursors provide high catalytic activity due to the high surface acidity, and high selectivity of diethylene glycol formation due to the "sieve effect" and concert acid-base mechanism of ethylene oxide addition.

STUDY OF SUPPORTED CATALYSTS SYNTHESIZED BY THE USE OF PLASMA TECHNIQUE

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Chem. Sustain. Devel., 11(1) (2003) pp. 233–238.

Some prospects of application of plasma spraying technique for the synthesis of supported catalysts are demonstrated. It was shown that Mn-containing catalysts deposited on γ-Al_2O_3 by means of plasma spraying demonstrate superior activity in methane oxidation reaction compared with those of reference catalysts prepared via standard conventional route.

Gradient alumina layer sprayed on the surface of metal supports of different geometry improves the performance characteristics of combustion catalysts on metal supports during long term operation at high temperatures.

A catalytic heat-exchanging (HEX) tubular reactor for combining exothermic combustion and endothermic methane steam reforming has been developed. The methane combustion and steam reforming catalysts were synthesized on the heat-conducting metal foam support materials by application of preliminary plasma spraying in order to increase adhesive properties of the active layer. The HEX reactor with perovskite or Pt supported catalyst on Ni-Cr foam material on the external surface of the HEX tube and with Ni containing reforming catalyst on the internal Ni foam was successfully tested in methane combustion reaction combined with methane steam reforming.

PLASMOCHEMICAL SYNTHESIS OF OXIDE CATALYSTS

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Phys. Mesomech., 6(2) (2003) pp. 127–132.

Plasma spraying technique is developed for synthesis of Mn-containing catalysts deposited on Al_2O_3. Significant phase, morphological and surface differences are detected between catalysts obtained by means of plasma spraying and reference catalysts prepared via standard conventional route.

These differences are shown to result in different catalyst performance in reaction of methane oxidation: catalysts, prepared by means of plasma spraying, provide higher catalytic activity compared with reference catalysts.

CHEMICAL COMPOSITION OF BORON CARBONITRIDE FILMS GROWN BY PLASMA-ENHANCED CHEMICAL VAPOR DEPOSITION FROM TRIMETHYLAMINEBORANE

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Inorg. Mater., 39(4) (2003) pp. 366–373.

Boron carbonitride and boron nitride films were grown by plasma-enhanced chemical vapor deposition using trimethylamineborane and its mixtures with ammonia, hydrogen, or helium. The effects of the starting-mixture composition and substrate temperature on the chemical composition of the deposits was studied by ellipsometry, scanning microscopy, IR spectroscopy, Raman scattering, and X-Ray photoelectron spectroscopy. The results indicate that the initial composition of the gas mixture, the nature of the activation gas, and substrate temperature play a key role in determining the deposition kinetics and the physicochemical properties of the deposits. Depending on these process parameters, one can obtain *h*-BN, *h*-BN + B_4C, or BC_xN_y films.

PLASMA-ENHANCED CHEMICAL VAPOR DEPOSITION OF SILICON CARBONITRIDE FILMS FROM VOLATILE SILYL DERIVATIVES OF 1,1-DIMETHYLHYDRAZINE

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High Energy Chem., 37(5) (2003) pp. 303–309.

Silicon carbonitride films were synthesized from new volatile precursors by plasma-enhanced chemical vapor deposition. Based on a detailed study of the morphology of film surfaces, it was found that the layer material was an amorphous matrix with inclusions of nanosized crystals. Calculation of the structure of the crystalline phase from synchrotron X-Ray diffraction patterns demonstrated that the entire set of the diffraction peaks detected is indexed by a tetragonal structure with the lattice parameters a = 9.6 Å and c = 6.4 Å. This is consistent with the fact that the carbon 1*s* and nitrogen 1*s* core level X-Ray photoelectron spectra exhibited only sp^3 bonding, which was expected for superhard carbon nitride phases.

COMPOSITION AND STRUCTURE OF FILMS DEPOSITED FROM SILYL DERIVATIVES OF ASYMMETRICAL DIMETHYLHYDRAZINE

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Inorg. Mater., 39(2) (2003) pp. 117–122.

Si–N–C films were produced by remote-plasma chemical vapor deposition using silyl derivatives of asymmetrical dimethylhydrazine as precursors and were characterized by optical spectroscopy, X-Ray photoelectron spectroscopy, scanning electron microscopy, and synchrotron X-Ray diffraction. The results demonstrate that Si–N and Si–C bonds prevail in the films deposited using excited hydrogen, while the structure of the films deposited using excited helium is dominated by Si–N and C–N bonds. The films contain both amorphous and crystalline silicon carbonitride. The crystalline phase can be indexed in a tetragonal cell with lattice parameters a = 9.6 Å and c = 6.4 Å. The formation of the crystalline phase and the shape of the crystallites are not correlated with the deposition temperature, which gives grounds to believe that the crystallization process may occur in the gas phase or on the film surface as a result of the increase in mechanical stress with increasing film thickness.

MICROSTRUCTURE AND CHEMICAL BONDING IN SILICON CARBONITRIDE FILMS SYNTHESIZED BY PLASMA ENHANCED CHEMICAL VAPOR DEPOSITION

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J. Struct. Chem., 44(1) (2003) pp. 169–173.

Silicon carbonitride films were synthesized by plasma enhanced chemical vapor deposition using silyl derivatives of asymmetric dimethylhydrazine, $(CH_3)_2HSiNHN(CH_3)_2$ and $(CH_3)_2Si[NHN(CH_3)_2]_2$, as molecular precursors. The film material consists of an amorphous matrix with nanocrystalline inclusions. Indexing of synchrotron radiation X-Ray diffraction patterns suggests that the structure of the nanocrystals is tetragonal with lattice parameters a = 9.6 Å and c = 6.4 Å. X-Ray photoelectron spectra indicate that Si—N and C—N sp^3 hybrid bonds are predominant. The absence of G- or D-modes in Raman spectra, which are otherwise typical of structures possessing sp^2 bonding, provides further support for the tetragonal structure of the nanocrystals.

SiCN ALLOYS OBTAINED BY REMOTE PLASMA CHEMICAL VAPOUR DEPOSITION FROM NOVEL PRECURSORS

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Thin Solid Films, 429 (1-2) (2003) pp. 144–151.

Silicon carbonitride films were synthesised in a remote plasma chemical vapour deposition process using novel single-source precursors $(CH_3)_2HSiNHN(CH_3)_2$ and $(CH_3)_2Si[NHN(CH_3)_2]_2$, which are silyl derivatives of 1,1-dimethylhydrazine. The films were characterised by X-Ray photoelectron (XPS), Fourier transform infrared (FTIR) and UV-VIS absorption spectroscopy. The microstructure of the films was examined by scanning electron microscopy and diffraction of synchrotron radiation methods. XPS and FTIR spectroscopic studies showed the Si—C and Si—N to be the basic bonds for the films deposited in the system with excited hydrogen, whereas the C—N and Si—N bonds are mainly peculiar to the films synthesised in the system with excited helium. The films were found to be predominately amorphous with a number of crystallites embedded in an unstructured matrix. The crystalline phase can be indexed in tetragonal cell with lattice parameters $a = 9.6$ Å and $c = 6.4$ Å. Appearance of the crystals, their dimensions and crystal forms did not depend on the substrate temperature. The crystallisation is hypothesised to be occurring either in the gas phase during deposition or in the solid as a result of the increase in mechanical stress with increasing film thickness. The FTIR and XPS data demonstrate the chemical bonding and the atomic local order in the amorphous matrix to be much more complicated than those of Si_3N_4-SiC or Si_3N_4-C_3N_4 mixtures. This novel material has an optical band gap varying within the energy range from 2.0 to 4.7 eV. The films obtained were highly resistant to thermal degradation.

ZIRCONIA PILLARED CLAYS: SYNTHESIS, CHARACTERIZATION AND CATALYTIC PROPERTIES IN THE NO_X SELECTIVE REDUCTION BY HYDROCARBONS IN THE OXYGEN EXCESS

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Chem. Sustain. Devel., 11(1) (2003) pp. 249–262.

Procedures for synthesis of thermally stable up to 750 °C zirconia-pillared clays (ZrPC) *via* intercalation of a montmorillonite clay with zirconium polyoxocations modified by cations of Ce, Fe, Al, Ca, Sr, Ba, were elaborated. Optimization of the preparation procedure allowed to obtain samples with specific surface area up to 300–400 m^2/g, the gallery height up to 10 Å and micropore volume up to 0.13 m^2/g. Active components comprised of copper cations and/or Pt clusters were supported on ZrPC by using photoassisted deposition. The structural and surface properties of pillars and effects of mutual interaction between the nanosized zirconia particles, and metal and oxide components were elucidated by using EXAFS, UV-VIS, ESR, H_2 TPR, NO_x TPD and FTIRS of adsorbed CO molecules. Catalytic properties of these systems were characterized in the reactions of NO_x selective reduction in the excess of oxygen by propane, propylene and decane. Strong interaction between the Pt atoms and copper cations resulted in substantial variation of the reactivity of the surface oxygen as well as bonding strength and coverages of surface ad-NO_x species. It was reflected in substantial improvement of the low-temperature activity of these systems as compared with those containing separate components. The nature of cation used for pillar modification was found to affect catalytic properties of supported active components, which can be explained by variation of the pillars structure and uniformity of their spatial distribution in clay galleries.

FUEL COMBUSTION REACTIONS AND CATALYSTS. 21. SYNTHESIS AND CHARACTERIZATION OF MODIFIED Mn-Al-O CATALYSTS FOR HIGH-TEMPERATURE OXIDATION

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Kinet. Catal., 44(6) (2003) pp. 806–812.

The phase composition of supported Mn–Al–O catalysts and their activity in the reaction of methane oxidation were studied depending on the composition of aluminum oxide supports (ν-Al_2O_3 with different χ-Al_2O_3 contents modified with individual Mg, La, and Ce oxides or Mg + La and Mg + Ce oxide mixtures) and calcination temperatures (500, 900, and 1300 °C). It was found that the Mn–Al–O catalysts based on ν-alumina containing χ-Al_2O_3 and modified with Mg, La, or Ce additives are more active and thermally stable (up to 1300 °C) than the samples based on pure ν-Al_2O_3. A conclusion was drawn that a higher degree of disorder of the structure of χ-Al_2O_3, compared to that of ν-Al_2O_3, is favorable for a deeper interaction of manganese and modifying additives with the support at the early stages of the synthesis and for the formation of Mn–Al compounds with complex composition (solid solutions and/or hexaaluminates) at 1300 °C. These compounds are responsible for the stability and high activity of the catalysts in methane oxidation

SYNTHESIS AND STUDYING OF PHYSICO-CHEMICAL PROPERTIES OF PEROVSKITES BASED ON STRONTIUM COBALTITE

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Proceed. Academy Sci., Physics, 67(7) (2003) pp. 951–953.

Data on synthesis and studying of physicochemical properties of perovskites based on strontium cobaltite, doped with niobium, are presented. It is shown that introduction of niobium results in structural disordering and stabilization of cubic perovskite structure and inhibiting of phase transitions due to expansion of the region of oxygen solid solutions existence.

THE EFFECT OF PREPARATION CONDITIONS ON THE PROPERTIES OF ALUMINOPLATINUM CATALYSTS OF DEEP OXIDATION

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Catal. Ind., 6 (2003) pp. 32-35.

The paper deals with the effect of the nature of platinum precursors and preparation conditions on the catalytic activity of catalysts for deep oxidation of methane and CO. The platinum precursors used in this work were H_2PtCl_6, $Pt(NO_3)_4$, and $H_2[Pt_3(CO)_6]_5$. The teta-alumina was used as a support. The catalysts are characterized by H_2-O_2-titration. It was shown that the catalysts prepared from platinum carbonyl precursor were more active for the both reactions. This effect is related to high platinum dispersity in these samples.

INFLUENCE OF TEMPERATURE ON THE AGGREGATION AND SEDIMENTATION RATE OF MONODISPERSE SPHERICAL SILICA PARTICLES

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React. Kinet. & Catal. Lett., 80(1) (2003) pp. 89–95.

The rise in temperature of alcohol suspensions of monodisperse silica particles to 50-100 °C results in an increase in the number of coagulated particles. This phenomenon results from an increase in the degree of electrolyte dissociation, which is equivalent to the rise in its concentration under normal conditions. The suspensions with the aggregates settle at elevated temperatures with the rates that are considerably higher than it is conditioned by the decrease in the viscosity of the suspension. The aggregates and free particles settle jointly, indicating that the non-aggregated particles are held in the field of the long-range molecular attraction of aggregates.

COMPOSITION AND MORPHOLOGY OF MAGNETIC MICROSPHERES IN POWER-PLANT FLY ASH OF COAL FROM THE EKIBASTUZ AND KUZNETSK BASINS

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Chem. Sustain. Devel., 11(4) (2003) pp. 639–648.

Using a multi-stage scheme including different sequences of the stages of magnetic separation, hydrodynamic and granulometric classification, magnetic microspheres of fixed composition containing the magnetic constituent at the level of 95-99 % were separated from the fly ash of coal from the Ekibastuz and Kuznetsk basins. The yield, texture characteristics, macrocomponent and mineral phase composition were determined and globules of three morphological types were described for close-cut fractions of magnetic microspheres. A general dependence of the properties of close-cut fractions of microspheres on ferric oxide content was revealed. It was demonstrated that for the mass concentration of total $Fe_2O_3 > 60$ %, mainly massive microspheres with various crystal microstructure are formed. With a decrease in iron content, the formation of porous microspheres becomes predominant. It is established that the governing factor in the formation of microspheres of morphological type is the viscosity of ferriferous silicate melt.

NATURAL COMPOUNDS IN THE SYNTHESIS OF CHIRAL ORGANOPHOSPHOROUS LIGANDS

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Russ. Chem. Rev., 72(9) (2003) 803–822.

Methods for the synthesis of chiral organophosphorus compounds based on natural optically active compounds (hydroxy acids, amino acids and their derivatives, mono- and disaccharides, mono- and diterpenoids, steroids) are discussed. Particular attention is given to the synthesis of bisphosphines and bisphosphinites. These compounds serve as ligands for transition metal complexes, which catalyze asymmetric hydrogenation. Data on the enantioselectivity of hydrogenation of unsaturated precursors of amino acids and unsaturated prochiral acids as well as on information on the enantioselectivity of hydrosilylation of ketones are surveyed (Bibliography includes 77 references).

DESIGN OF THE SURFACE OF PARTICLES IN THE EMULSION POLYMERIZATION OF METHYL METHACRYLATE IN THE PRESENCE OF CARBOXYLATED DEXTRAN DERIVATIVES

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Polym. Sci., A, 45(4) (2003) pp. 380–385.

It was shown that carboxylated dextran derivatives used as polymer stabilizers can significantly accelerate the emulsion polymerization of methyl methacrylate initiated by 4,4'-azo-bis (4-cyanisovaleric acid). It was proposed that the process proceeds via the microemulsion mechanism. By varying the structure of a dextran derivative and its concentration in the reaction mixture, one can accomplish the targeted design of submicron monodisperse particles and can influence the structure of their surface. Using the microelectrophoresis method, it was established that the surface carboxyl groups located on polysaccharide chains exhibit an enhanced mobility. The adsorption and covalent binding of a protein by the surface of the obtained particles were studied, and their efficiency as adjuvant immunoreagent carriers was demonstrated.

Catalysis on Zeolites

DEACTIVATION BY COKING AND REGENERATION OF ZEOLITE CATALYSTS FOR BENZENE-TO-PHENOL OXIDATION

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Appl. Catal., A, 241(1–2) (2003) pp. 113–121.

The object of the study was to determine the effect of coke, formed in the nitrous oxide oxidation of benzene-to-phenol (BTOP), on the catalytic and texture properties of ZSM-5. The study was conducted on three series of catalyst samples. The samples of the first series were withdrawn from the benzene oxidation reactor after different amount of time-on-stream. The samples of the second series were obtained by partial regeneration of coked zeolite with O_2. Finally, the samples of the third series were similar to the second series, except in this case they were partially regenerated with N_2O. Catalytic activity and concentration of active sites on the samples of the first series linearly decreased with the increase of coke content. Catalytic activity of partially regenerated samples was not directly proportional to the coke amount on a sample. In the case of catalyst regeneration with nitrous oxide, a complete restoration of catalytic activity required the removal of only 30–35 % coke. In the case of regeneration in oxygen, catalytic activity was fully restored after removal 60–65 % of the total coke amount. Despite these differences, the dependence of catalytic activity on active site concentration appeared to be the same for all samples of the three series; catalytic activity was directly proportional to the concentration of active sites. This indicates that the activity of a single site is constant regardless of coke content and the method of coked sample preparation. The deactivating effect of coke is caused by poisoning of these sites.

KINETICS OF BENZENE TO PHENOL OXIDATION OVER Fe-ZSM-5 CATALYST

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Appl. Catal., A, 249(2) (2003) pp. 327–343.

Benzene to phenol oxidation by nitrous oxide over the Fe-ZSM-5 catalyst was studied at 648–698 K and near atmospheric pressure using a bench scale plug flow reactor with a feed gas concentration of

30–80 mol % benzene, 1.5–5.0 mol % N_2O, and 0–4.7 mol % phenol. At these conditions, the selectivity of benzene and N_2O to phenol exceeded 98 and 95 %, respectively. Benzoquinone, hydroquinone, catechol, and carbon oxides were the main by-products. The rate of N_2O consumption was observed to be first order with respect to N_2O concentration, and was observed to decrease with increasing benzene and phenol concentration. The apparent activation energy was 126 kJ/mol. A sorption kinetic model was developed. It was assumed that benzene and phenol are in sorption equilibrium between the gas-phase and the zeolite micropore volume. The limiting step of the overall reaction sequence is the reaction between sorbed N_2O and catalyst active sites bound with phenol. The interaction of sorbed benzene and phenol with oxidized α-sites is relatively fast. The equilibrium constant for benzene sorption on ZSM-5 was estimated from the kinetic data and was found to be in a good agreement with the sorption measurements reported in the literature. It was observed that the ratio of the specific rate of phenol formation to the specific rate of dihydroxybenzene formation is independent of temperature.

COMPETING MICHAEL AND KNOEVENAGEL REACTIONS OF TERPENOIDS WITH MALONONITRILE ON BASIC Cs-BETA ZEOLITE

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J. Mol. Catal. A: Chem., 195(1–2) (2003) pp. 263–274.

The synthesized basic Cs-beta zeolite has been shown to be an effective catalyst for reactions of a number of terpenoid α, β-unsaturated carbonyl compounds with malononitrile leading to products of either Michael or Knoevenagel reactions or both.

Basic cesium-beta (Cs-beta) zeolite has been synthesized. It proved to be an effective catalyst in reactions of a number of α, β-unsaturated carbonyl compounds with malononitrile. It is shown that the process is either the Michael or Knoevenagel reaction, or tandem transformations generally initiated by the Michael reaction, which depends on steric hindrance at the carbonyl group and the β-position of the carbon = carbon (C = C) double bond adjacent to the carbonyl group.

Carbon and Carbon Related Catalytic Processes

CATALYTIC FILAMENTOUS CARBON: STRUCTURAL AND TEXTURAL PROPERTIES

T.V. Reshetenko, L.B. Avdeeva, Z.R. Ismagilov, V.V. Pushkarev*, S.V. Cherepanova, A.L. Chuvilin, V.A. Likholobov (*Department of Chemical and Petroleum Engineering, University of Pittsburgh, Pittsburgh, USA)

Carbon, 41(8) (2003) pp. 1605–1615.

Catalytic filamentous carbon (CFC) synthesized by the decomposition of methane over iron subgroup metal catalysts (Ni, Co, Fe or their alloys) is a new family of mesoporous carbon materials possessing the unique structural and textural properties. Microstructural properties of CFC (arrangement of the graphite planes in filaments) are shown to depend on the nature of catalyst for methane decomposition. These properties widely vary for different catalysts: the angle between graphite planes and the filament axis can be 0° (Fe–Co–Al_2O_3), 15° (Co–Al_2O_3), 45° (Ni–Al_2O_3), 90° (Ni–Cu–Al_2O_3). The textural properties of CFC depend both on the catalyst nature and the conditions of methane decomposition (*T*, °C). The micropore volume in CFC is very low, 0.001-0.022 cm^3g^{-1} at the total pore volume of 0.26–0.59 cm^3g^{-1}. Nevertheless, the BET surface area may reach 318 m^2g^{-1}. Results of the TEM (HRTEM), XRD, Raman spectroscopic, SEM and adsorption studies of the structural and textural properties of CFC are discussed.

DETAILED STRUCTURE OF THE HEXAGONALLY PACKED MESOSTRUCTURED CARBON MATERIAL CMK-3

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Carbon, 40(13) (2002) pp. 2477–2481.

Detailed investigation of the ordered mesoporous CMK-3 carbon using XRD structural modeling based on the continuous electron density representation and the

Rietveld technique allowed deriving comprehensive and consistent information on the material anatomy. The electron density distribution map agrees with carbon 'bridges', which seem to be attributed to the material interconnecting carbon nanorods in the CMK-3 mesostructure. These carbon 'bridges' are supposed to be derived from former complementary mesopores of the SBA-15 template used.

FRAMEWORK CHARACTERIZATION OF MESOSTRUCTURED CARBON CMK-1 BY X-RAY POWDER DIFFRACTION AND ELECTRON MICROSCOPY

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J. Phys. Chem. B, 106(47) (2002) pp. 12198–12202.

The model of structure and structural transformation of the mesostructured carbon material CMK-1 was established by X-Ray powder diffraction (XRD) and transmission electron microscopy (TEM) investigations. The investigations showed that the enantiomeric carbon subframeworks formed within the pores of the MCM-48 mesoporous template used for the material synthesis displaced with respect to one another without significant distortions after the dissolution of the silica wall of the template. The model proposed agrees well with TEM images observed. The XRD structural modeling of CMK-1 done using the continuous density function technique allowed perfect fit of the calculated to the experimental powder diffraction pattern and provided geometric characteristics of the material texture. The structural characteristics obtained agreed fairly well with TEM analysis and with previously reported adsorption data.

PREPARATION OF MICROPOROUS SORBENTS FROM CEDAR NUTSHELLS AND HYDROLYTIC LIGNIN

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Carbon, 41(9) (2003) pp. 1793–1800.

Carbon nutshells and hydrolytic lignin were used as starting materials for the preparation of microporous active carbons. Optimum parameters for cedar nutshell carbonization have been selected (temperature of carbonization 700–800 °C, rate of heating less than 3 °C/min) for the preparation of microporous carbons (average pore width 0.56 nm). The textural characteristics of microporous carbons made from nutshell are similar to those of a ‘Coconut’ carbon molecular sieve, but the latter has both a higher CO_2 adsorption capacity and a higher coefficient of N_2/O_2 separation. The influence of carbonization and steam-activation parameters on the microtexture and molecular-sieve properties of granular carbons made from hydrolytic lignin was also investigated. A low rate of heating (less 3°C/min) promotes the formation of micropores with average sizes around 0.56–0.58 nm at carbonization temperature 700 °C. At the same carbonization temperature the average sizes of micropores were 0.7–0.78 nm at rates of heating more than 3 °C/min. The activation of lignin-char with steam at 800 °C resulted in the formation of active carbons with more developed micropore volume (0.3–0.35 cm^3 g^{-1}) and with micropores of widths around 0.6–0.66 nm which are able to separate He from a He–CH_4 mixture. The size of the micropores was varied as a function of burn off value.

SULFUR DISTRIBUTION ON THE SURFACE OF MESOPOROUS NANOFIBROUS CARBON

V.V. Shinkarev, V.B. Fenelonov, G.G. Kuvshinov

Carbon, 41(2) (2003) pp. 295–302.

Distribution of sulfur in the mesoporous carbon catalysts for the direct selective oxidation of hydrogen sulfide has been investigated. Granules of carbon nanofibers, produced by catalytic pyrolysis of methane on the heavily loaded nickel and copper–nickel catalysts were used as catalysts. It was established that sulfur deposits similar to the adsorbates which actively interact with the adsorbent surface via the typical mechanism of physical adsorption, involving the filling of micropores at low sorption degrees with consequent formation of a single-layered coverage on the rest surface. A method for studying such distribution is proposed.

EFFECT OF THE NATURE OF COKE-FORMING SPECIES ON THE CRYSTALLOGRAPHIC CHARACTERISTICS AND CATALYTIC PROPERTIES OF METAL-FILAMENTOUS CARBON CATALYSTS IN THE SELECTIVE HYDROGENATION OF 1,3-BUTADIENE

N.A. Zaitseva, V.V. Molchanov, V.V. Chesnokov, R.A. Buyanov, V.I. Zaikovskii

Kinet. Catal., 44(1) (2003) pp. 129–134.

The particle morphology and surface structure of nickel metal in metal–filamentous carbon catalysts were found to depend on the nature of coke-forming species used in the synthesis of catalysts. Metal carbonization with hydrocarbons that are characterized by high thermodynamic stability results in the formation of well-cut metal particles the surface of which is formed by (110) facets. Selective hydrogenation reactions of diene and acetylene hydrocarbons to olefins are typical of these catalysts. In the catalytic decomposition of hydrocarbons with relatively low thermodynamic stability, metal particles become irregular in shape, and their surface is formed by (111) facets. In this case, the reactions of full hydrogenation of olefin, diene, and acetylene hydrocarbons to corresponding alkanes take place. These data are consistent with the found dependence of the catalytic properties of catalysts on the character of the exterior faceting of active metal particles.

STATE OF THE ACTIVE COMPONENT AND CATALYTIC PROPERTIES OF Pd/C CATALYSTS ON THE SELECTIVE HYDROGENATION OF BUTADIENE-1,3 INTO BUTYLENES

V.V. Chesnokov, I.P. Prosvirin, V.I. Zaikovskii, N.A. Zaitseva

Eurasian Chem.-Tech. J.,
5(2) (2003) pp. 127–136.

Palladium (0.25-5.8 wt. %) was supported on three different types of filamentous carbon in which the basal graphite planes are arranged along, crosswise and at a 45° angle to the axis of a nanofiber. HREM, XPS and X-Ray techniques were used to study the state of highly dispersed Pd particles supported on the filamentous carbon. It was established that the type of the carbon support affects the properties of the active component. The highly dispersed Pd particles most strongly interact with the prismatic planes of graphite to provide electron transfer from palladium to the support, which stabilizes palladium in a more dispersed state. Because of this strong interaction, Pd^{2+} is stabilized in the ionic state. A change in the properties of the palladium particles initiates changes in the catalytic properties of Pd/C catalysts in the reaction of selective hydrogenation of 1,3-butadiene into butylenes. An increase in the fraction of Pd^{2+} in the catalyst composition results in the decrease of both total activity and selectivity of Pd/C catalysts in the considered reaction.

CARBON CAPACIOUS Ni-Cu-Al_2O_3 CATALYSTS FOR HIGH-TEMPERATURE METHANE DECOMPOSITION

T.V. Reshetenko, L.B. Avdeeva, Z.R. Ismagilov, A.L. Chuvilin, V.A. Ushakov

Appl. Catal., A, 247(1) (2003) pp. 51–63.

Steady and efficient decomposition of methane can be achieved at 625–675 °C over copper-promoted (8–15 wt. % of copper) nickel catalysts prepared from a Feitknecht compound precursor. Such catalysts permit one to increase the yield of catalytic filamentous carbon (CFC) and control both microstructural and textural properties of CFC by varying the copper concentration in the catalyst. The maximal conversion of methane into hydrogen and carbon reaches 40 % at 675 °C at the carbon capacity not lower than 700 g/g_{Ni} under optimal conditions. The BET surface area of the CFC is 285.9 m^2/g. The influence of promotion of nickel-containing catalysts with copper on the catalytic activity is discussed.

PROMOTED IRON CATALYSTS OF LOW-TEMPERATURE METHANE DECOMPOSITION

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Chem. Sustain. Devel.,
11(1) (2003) pp. 239–247.

Iron-containing catalysts promoted by nickel or cobalt were tested in methane decomposition reaction at low temperature (600–650 °C) and pressure 1 bar in order to study their catalytic properties and to produce catalytic filamentous carbon (CFC). Catalyst preparation method and composition of the catalysts were found to influence their properties. It was found that introduction of cobalt or nickel in small amount (3–10 % mass) results in the magnification of carbon yields 2–3 times in comparison with Fe-Al_2O_3.

Investigations of Fe-Co-Al_2O_3 and Fe-Ni-Al_2O_3 catalysts genesis were performed by Mössbauer spectroscopy, XRD, TEM. It is established that Co or Ni additives render activating influence on Fe catalysts, which become apparent in decrease of the methane decomposition temperature and the formation of multiwall carbon nanotubes (MWNTs).

Ni/SiO_2 AND Fe/SiO_2 CATALYSTS FOR PRODUCTION OF HYDROGEN AND FILAMENTOUS CARBON VIA METHANE DECOMPOSITION

M.A. Ermakova, D.Yu. Ermakov

Catal. Today, 77(3) (2002) pp. 225–235.

High-loaded Ni–SiO_2 and Fe–SiO_2 catalysts (85–90 wt. % of metal) for methane decomposition were prepared by the heterophase sol–gel method and studied at various stages of their preparation and operation using XRD, IR, TPR, TEM techniques and the stoichiographic method of differentiating dissolution. Carbon yield was demonstrated to depend on the interaction between nickel and silica. The yield equal to 384 gC/g_{Ni} was characteristic of the catalyst free of silicates, while the presence of silicates in amount of 1.5–2 wt. % caused a decrease in the carbon yield to 40 gC/g_{Ni}. The effect of silicates comprised in iron catalysts is not so unambiguous as for nickel catalysts, they can both inhibit and promote the process of carbon formation.

EFFECT OF INTERACTIONS BETWEEN COMPONENTS IN NICKEL-SILICA CATALYSTS ON THE YIELD OF CARBON IN METHANE DECOMPOSITION

M.A. Ermakova, D.Yu. Ermakov

Kinet. Catal., 44(2) (2003) pp. 268–278.

A number of 90% Ni–10 % SiO_2 catalysts for methane decomposition were studied at different stages of preparation and operation in the reaction using X-Ray diffraction analysis, differential dissolution, temperature-programmed reduction, IR spectroscopy, and high-resolution electron microscopy. It was found that an increase in the interaction between components in the catalytic system decreased the ability of nickel to accumulate carbon in the decomposition of methane.

TEM EVIDENCE FOR FACTORS AFFECTING THE GENESIS OF CARBON SPECIES ON BARE AND K-PROMOTED Ni/MgO CATALYSTS DURING THE DRY REFORMING OF METHANE

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Carbon, 40(7) (2002) pp. 1063–1070.

The structure and morphology of carbon species generated under dry reforming of methane (DRM) at 650 and 800 °C on 'bare' and 'K-doped' Ni/MgO catalysts have been comparatively investigated by Transmission Electron Microscopy (TEM) analyses of 'used' samples. K-addition (K_{at}/Ni_{at}, 0.125) strongly improves the resistance of the Ni/MgO catalyst to coking and sintering phenomena at any temperature. At 650 °C, an extensive formation of filamentous (whisker carbon) carbon species on bare Ni/MgO catalyst causes the detachment of a large number of Ni particles from the support with a consequent destruction of the structure and remarkable sintering phenomena of the active phase. Considerably lower amounts of carbon deposits with a shell-like (encapsulating carbon) morphology, forming at 800 °C on both catalysts, point to the Bouduard reaction as the main route of carbon deposition on Ni-based catalysts during DRM. The electronic effect induced by potassium on the active phase of the Ni/MgO system, timely monitored by a rise in E_{app} of DRM from 50 to 70 kJ/mol, markedly hinders the rate of coking also affecting the morphology of carbon whiskers, by inhibiting the processes of C diffusion and nucleation across Ni particles under steady-state conditions.

FORMATION MECHANISM AND STRUCTURE OF MONATOMIC CARBON FILMS IN ETHYLENE DECOMPOSITION ON THE Pt(111) SURFACE ACCORDING TO XPS DATA

E.M. Pazhetnov, S.V. Koscheev, A.I. Boronin

Kinet. Catal., 44(3) (2003) pp. 414–419.

The interaction of ethylene with a Pt(111) single-crystal surface was studied using X-Ray photoelectron spectroscopy. It was found that both two-dimensional flat graphite islands and curved fullerene-like carbon structures or nanotubes can be formed depending on the reaction temperature of ethylene and the presence of dissolved carbon in the bulk of the crystal. It was assumed that the size and curvature of the islands depend on the size of terraces on the single-crystal surface.

MECHANISM OF COKING ON METAL CATALYST SURFACES.

1. THERMODYNAMIC ANALYSIS OF NUCLEATION

V.L. Kuznetsov, A.N. Usoltseva, Yu.V. Butenko

Kinet. Catal., 44(5) (2003) pp. 726–733.

Thermodynamic analysis of carbon nucleation on a metal surface is carried out. The fundamental equation is obtained that relates the critical radius of a nucleus and reaction parameters, such as temperature, metal particle oversaturation by carbon, the work of metal adhesion to graphite, and the metal–carbon bond energy. The results are compared with experimental data and conditions for the formation of carbon deposits of various kinds on metal particles are analyzed. A new mechanism for the formation of carbon nanotubes with a "bamboo" structure is proposed. This mechanism is based on a periodical change in the degree of metal particle oversaturation by carbon. The optimal conditions for the synthesis of single-wall nanotubes are formulated.

THE INFLUENCE OF INERT IMPURITIES ON THE CATALYST LIFETIME AND PROPERTIES OF NANOFIBROUS CARBON PRODUCED BY UTILIZATION OF DILUTED HYDROCARBON GASES

G.G. Kuvshinov, D.G. Kuvshinov, A.M. Glushenkov

Chem. Sustain. Devel.,
11(1) (2003) pp. 135–140.

Experimental studies were focused on the feasibility of utilization of hydrocarbons diluted with inert gases (such as associated oil gases) during the synthesis of nanofibrous carbon. The carbon yield and catalyst lifetime was studied regarding the initial reaction mixture parameters. Varying the composition of the initial gas mixture, it is possible to control textural characteristics of the resulting carbon product.

ADSORPTION METHODS OF HYDROGEN AND METHANE STORAGE FOR THE FUEL CELL APPLICATION

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Eurasian Chem.-Tech. J.,
5(1) (2003) pp. 19–28.

Adsorption of H_2 and CH_4 was performed at a pressure up to 100 atm on the samples of catalytic filamentous carbon (CFC) and supermicroporous active carbon (SAC) with a surface area ca. 3000 m^2/g. It is shown that H_2 is better sorbed on the CFC than on the SAC, while the opposite is observed for the CH_4 adsorption. The high values of H_2 sorption on the CFC (to 25-35 mg H_2/g carbon) with a surface area of 100-300 m^2/g is explained by hydrogen intercalation between the graphite-like CFC layers. Thus, it is worthwhile investigating the possibility of hydrogen and methane storage on the carbon porous materials.

Fe NANOWIRES IN CARBON NANOTUBES AS AN EXAMPLE OF A ONE-DIMENSIONAL SYSTEM OF EXCHANGE-COUPLED FERROMAGNETIC NANOPARTICLES

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JETP Letters, 78(4) (2003) pp. 236–240.

The cooperative phenomena revealed in the field and temperature dependencies of the magnetization in a system of iron nanoparticles in carbon nanotubes were studied experimentally. The character of the temperature dependencies of the magnetization indicates that the ferromagnetic Fe particles in carbon nanotubes are exchange-coupled. In the region where the magnetization approaches saturation, the magnetization curves reveal the power dependence $\Delta M \sim H^{-3/2}$ typical for a one-dimensional system of exchange-coupled ferromagnetic nanoparticles.

PHOTOEMISSION SPECTROSCOPY OF CLEAN AND POTASSIUM-INTERCALATED CARBON ONIONS

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(*University of Newcastle upon Tyne, Newcastle upon Tyne, UK; **CCLRC, Daresbury Laboratory, Warrington, Cheshire, UK; ***Surface Science Centre, Liverpool University, Liverpool, UK; ****University of Nottingham, University Park, Nottingham, UK)

Phys. Rev. B: Condens. Matter,
67(11) (2003) 113401.

Hollow onionlike carbon (OLC), generated by annealing nanodiamond at 2140 K, has been studied by core-level and valence-band photoemission spectroscopy. Upon intercalation with potassium, core and valence states of the OLC show an almost rigid shift to higher binding energies, and the density of states at the Fermi level (E_F) is observed to increase. An asymmetric broadening of the C1*s* line from the OLC as intercalation proceeds indicates an increase in electron-hole pair excitations. Both core and valence-band spectra are consistent with charge transfer from the intercalated potassium to the OLC, and support the conclusion that the electronic structure of the carbon onions bears strong similarity to that of graphite, although differences do exist. In consequence the conclusion can be drawn that these species behave as graphite "nanocrystals" rather than as large fullerene molecules.

Studies on Metal Catalysts

SELECTIVE OXIDATION OF CARBON MONOXIDE IN EXCESS HYDROGEN OVER Pt-, Ru- AND Pd-SUPPORTED CATALYSTS

P.V. Snytnikov, V.A. Sobyanin, V.D. Belyaev, P.G. Tsyrulnikov, N.B. Shitova, D.A. Shlyapin

Appl. Catal. A: General,
239(1-2) (2003) pp. 149–156.

Selective oxidation of CO in excess hydrogen has been studied over Pt-, Ru- and Pd-supported on Sibunit (porous carbonaceous material) catalysts. The Ru and Pt catalysts were found to be the most active and selective among the studied catalysts. They provided single-step removal of CO from hydrogen-rich stream both in the absence and presence of CO_2 and H_2O to a PEMFC tolerant level.

MONOMETALLIC AND BIMETALLIC Pt- AND Ru-BASED CATALYSTS FOR SELECTIVE OXIDATION OF CO IN EXCESS HYDROGEN

P.V. Snytnikov, V.A. Sobyanin, V.D. Belyaev, D.A. Shlyapin

Chem. Sust. Devel., 11(1) (2003) pp. 297–301.

Selective oxidation of CO in excess hydrogen and in the presence of CO_2 and H_2O has been studied over monometallic Pt, Ru and bimetallic Pt–Ru supported on porous carbonaceous material catalysts. The catalysts provided CO conversion ≥ 98 % and seem to be promising for efficient single-step removal of CO from hydrogen-rich streams containing CO_2 and H_2O.

MECHANISM FOR CO OXIDATION AND OSCILLATORY REACTIONS ON Pd TIP AND Pd(110) SURFACES: FEM, TPR, XPS STUDIES

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Chem. Sust. Devel., 11(1) (2003) pp. 67–75.

Detailed studies of the coadsorption of oxygen and carbon monoxide, hysteresis phenomena and oscillatory reaction of CO oxidation on Pd(110) and Pd tip surfaces have been carried out with the molecular beam (MB), field electron microscope (FEM), temperature programmed reaction (TPR) and X-Ray photoelectron spectroscopy (XPS). It has been found that the occurrence of kinetic oscillations over Pd surfaces is associated with periodic formation and depletion of subsurface oxygen (O_{sub}). Transient kinetic experiments show that CO does not react chemically with subsurface oxygen to form CO_2 below 300 K. It has been found that CO does react with an atomic O_{ads}/O_{sub} state beginning at temperature ~150 K. Analysis of Pd tip surface with a local resolution of ~20 Å shows the availability of a sharp boundary between the mobile CO_{ads} and O_{ads} fronts.

INFLUENCE OF OXYGEN ADSORPTION ON SURFACE EXPLOSION PHENOMENA IN THE NO+CO/Pd(110) SYSTEM

A.V. Matveev, A.A. Sametova, N.N. Bulgakov, V.V. Gorodetskii

Chem. Sustain. Devel., 11(1) (2003) pp. 181–188.

In the present work adsorption of NO and coadsorption of NO, CO and O_2 has been investigated by means of thermal desorption spectroscopy (TDS) and temperature programmed reaction (TPR). Influence of adsorbed oxygen on morphology of Pd-nanoparticles as well as Pd(110) plane was studied by the theoretical Method of Interacting Bonds. It has been shown that adsorption of atomic oxygen induces the morphology changes of Pd-nanocrystals and Pd(110) plane. By analysis of TPR spectra of desorbing N_2 and CO_2 for different NO_{ads} + CO_{ads} coverages, an autocatalytic reaction in an "explosive" way was suggested. The addition of oxygen was found to inhibit the process of NO dissociation. Exposure of NO and CO on oxygen pre-adsorbed layer results in appearing of low-temperature peak of CO_2 in TPR spectra at 265 K.

CO OXIDATION OVER THE Pt-Rh SYSTEM.
2. REACTION ON AN ALLOY

A.V. Kalinkin, A.V. Pashis, V.I. Bukhtiyarov

React. Kinet. Catal. Lett.,
78(1) (2003) pp. 107–112.

The oxidation of CO over thin films of a Pt-Rh alloy prepared by sequential vacuum evaporation of the metals on an inert support has been investigated at low pressures ($P < 2{\cdot}10^{-5}$ mbar). The results are compared with the data on the individual surfaces of Pt and Rh. It is found that the activity of the alloy is intermediate between the activities of the individual metals. The effect of alloy formation on the catalytic activity in CO oxidation is discussed.

CO OXIDATION OVER THE Pt-Rh SYSTEM.
3. REACTION ON A HETEROPHASE SURFACE

A.V. Kalinkin, A.V. Pashis, V.I. Bukhtiyarov

React. Kinet. Catal. Lett.,
78(1) (2003) pp. 121–127.

The reaction of the CO oxidation over a Pt-Rh heterophase surface, which represents 10-20 nm platinum particles located on a rhodium film, which in turn is deposited on an inert support, has been investigated at low pressures ($P < 2{\cdot}10^{-5}$ mbar). The results are compared with the data for the clean surfaces of Pt and Rh. In the high-temperature range, the rate of CO_2 formation on the heterophase surface is found to be higher than the sum of the rates on individual metals corrected by the surface area of the different metals. The nature of the synergistic effect in the CO oxidation is discussed.

Pt-CONTAINING CATALYSTS ON A BASE OF WOVEN GLASS FIBER SUPPORT: A NEW ALTERNATIVE FOR TRADITIONAL VANADIUM CATALYSTS IN SO_2 OXIDATION PROCESS

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Chem. Eng. J., 91(2-3) (2003) pp. 175–179.

Pt-containing catalysts (0.01–0.12 % Pt), supported on leached sodiumsilicate glass fiber were tested in sulfur dioxide oxidation (10–20 % SO_2) at 420–700 °C. Catalysts showed high activity and good thermal resistance.

TEXTURE AND CATALYTIC PROPERTIES OF PALLADIUM SUPPORTED ON THERMALLY EXPANDED NATURAL GRAPHITE

B.N. Kuznetsov*, N.V. Chesnokov*, N.M. Mikova*, V.I. Zaikovskii, V.A. Drozdov, M.V. Savos'kin, A.M. Yaroshenko**, S.B. Lyubchik**** (*Institute of Chemistry and Chemical Technology, Krasnoyarsk, Russia; **Institute of Physical Organic and Coal Chemistry, Donetsk, Ukraine)

React. Kinet. Catal. Lett.,
80(2) (2003) pp. 345–350.

Data about preparation and properties of palladium catalysts on porous supports prepared by intercalation and subsequent thermal expansion of natural graphite are presented. Some relations between the structure of the graphite support, the state of supported palladium and its catalytic properties in the model reaction of cyclohexene liquid-phase hydrogenation were established.

MODIFICATION OF THE SUPPORTED PALLADIUM CATALYSTS SURFACE DURING HYDRODECHLORINATION OF CARBON TETRACHLORIDE

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Appl. Catal. A: General, 241(1-2) (2003) pp. 123–132.

Hydrodechlorination (HDC) of carbon tetrachloride (CCl_4) was studied in the presence of 0.5–5 % palladium catalysts supported on carbon material Sibunit and TiO_2. Experiments were performed in a flow-type reactor in hydrogen at 150–220 °C. Non-chlorinated C_1–C_5 hydrocarbons were formed in the presence of all catalysts. Stable work (more than 4h) was observed in the most cases. Conversion of carbon tetrachloride was 100 %. It was assumed, that Cl, which was formed as intermediate during dissociative adsorption of CCl_4, oxidizes palladium on the catalytic surface generating active sites of oligomerization. The surface of the catalyst is covered by carbonaceous deposits during the HDC, resulting in deactivation of the catalyst. These deposits are probably a little different in nature for Pd/Sibunit and Pd/TiO_2 catalysts. For Pd/Sibunit carbonaceous deposits are more hydrocarbonaceous in nature. These carbonaceous deposits can be removed by heating in argon-flow to regenerate the catalyst.

Catalysis by Sulfide Catalysts

STRUCTURE AND THIOPHENE HYDRODESULFURIZATION ACTIVITY OF MoS_2/Al_2O_3 CATALYSTS

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Kinet. Catal., 44(1) (2003) pp. 135–140.

It was found that, in MoS_2/Al_2O_3 catalysts prepared by exfoliation, the structure of MoS_2 is strongly distorted. The catalytic activities of these catalysts and traditionally prepared catalysts toward the hydrodesulfurization of thiophene were compared. It was established that the stacking dimension of MoS_2 in the catalysts prepared by exfoliation was 200 Å, whereas it was 20 Å in a standard catalyst. It was demonstrated that, although the number of molybdenum atoms in the edge plane per gram of MoS_2 in the catalysts prepared by exfoliation was 10 times smaller than that in the standard catalyst, the activity of these catalysts was close to the activity of the standard catalyst. On this basis, it was suggested that the hydrodesulfurization of thiophene can occur on the basal plane of MoS_2 that has a defect-free structure with a distorted environment of molybdenum.

THIOPHENE HYDROGENATION TO TETRAHYDROTHIOPHENE OVER TUNGSTEN SULFIDE CATALYSTS

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Kinet. Catal., 44(2) (2003) pp. 277–282.

Independent reactions of thiophene reduction to tetrahydrothiophene and thiophene hydrogenolysis to form hydrogen sulfide and C_4 hydrocarbons are shown to occur over supported tungsten sulfide catalysts and unsupported tungsten sulfide at an elevated temperature and a high pressure. The highest rate of tetrahydrothiophene formation over the supported catalysts is observed when alumina was used as a support, and the lowest reaction rate is found when silica gel was used as a support. Both catalysts are less active than unsupported tungsten disulfide. The rate of thiophene hydrogenation over tungsten disulfide increases with increasing thiophene concentration and hydrogen pressure and is inhibited by tetrahydrothiophene. The selectivity to tetrahydrothiophene is constant (70–90 %) in the whole range up to high thiophene conversions. The high selectivity over tungsten sulfide catalysts is suggested to be due to the reaction pathway through thiophene protonation mediated with the surface SH groups and to the inhibition of hydrogenolysis.

SULFIDE HYDRODESULFURISATION CATALYSTS: STRUCTURE OF THE ACTIVE COMPONENT AND MECHANISM OF THE CATALYTIC ACTION

A.N. Startsev, I.I. Zakharov

Russ. Chem. Rev., 72(6) (2003) pp. 517–536.

A new phenomenon in heterogeneous catalysis, namely, oxidative addition of hydrogen to active metal atoms (Ni, Co) within sulfide catalysts for hydrodesulfurisation, is considered. The possibility of hydrogen occlusion into the MoS_2 matrix of the active component of the catalysts is demonstrated. The electronic structure of Ni(IV) and Co(III) active centres with d^6 electron configuration is analyzed. A concerted mechanism of thiophene hydrogenolysis on a bimetallic active site is considered and substantiated. The concept of the governing role of the metal–sulfur bond energy in catalysis by metal sulfides is critically analyzed (Bibliography — 198 references).

AN UNEXPECTED PHENOMENON IN HETEROGENEOUS CATALYSIS: OXIDATIVE ADDITION OF HYDROGEN TO THE SULFIDE CATALYSTS

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J. Mol. Catal. A: Chem.,
192(1–2) (2003) pp. 113–127.

The paper summarizes experimental and theoretical evidence of an oxidative addition of hydrogen to the active metal (Ni or Co) in the active component of the sulfide HDS catalysts — a new phenomenon unknown to date in heterogeneous catalysis. Several aspects are discussed: thermodynamics of the oxidative addition of hydrogen; possible mechanism of dihydrogen activation by sulfide catalysts; electronic state of the active metals Ni(IV) and Co(III) with d^6-electron configuration; reversibility of the oxidative addition and reductive elimination of hydrogen at high temperature; sites of hydrogen localization inside the active component matrix; spectroscopic evidence on the existence of “occluded” hydrogen; a strong interaction of the occluded hydrogen with the active component matrix; a new version of the catalytic cycle of thiophene hydrogenolysis.

HYDROGEN OCCLUDED IN SULFIDE CATALYSTS: EVIDENCE FROM THE TEMPERATURE PROGRAMMED HEATING TECHNIQUE

A.E. Shalagina, G.I. Aleshina, A.N. Startsev

React. Kinet. Catal. Lett.,
78(1) (2003) pp. 91–98.

Strongly bonded hydrogen is found in alumina supported sulfide Co, Ni, Mo, (Co, Mo) and (Ni, Mo) catalysts. This hydrogen is desorbed from the catalysts in the temperature range of 500–750 °C and seems to be occluded in the corresponding sulfide matrix. Possible sites of its localization in the sulfide crystal lattice are discussed.

Catalysis by Metal Complexes and Heteropolycomplexes

INTERACTION OF MOLYBDOPHOSPHATES WITH PALLADIUM(II) SALTS IN AQUEOUS SOLUTION

L.G. Detusheva, L.I. Kuznetsova, M.A. Fedotov, L.S. Dovlitova, A.A. Vlasov, V.A. Likholobov, V.V. Malakhov

Russ. J. Inorg. Chem.,
48(1) (2003) pp. 1685–1690.

UV-VIS spectroscopy and ^{31}P NMR spectroscopy were used to study the interaction of $H_3PMo_{12}O_{40}$ with H_2PdCl_4 or $PdSO_4$ in aqueous solution at pH 3.0–4.5 and the ratio $[Pd(II)] : [H_3PMo_{12}O_{40}] = 1 : 1$. Palladium(II) remains in solution in the form of intensely colored hydroxo species and does not change the structure of the newly formed unsaturated heteropoly molybdates $PMo_{11}O_{39}^{7-}$ and $PMo_9O_{34}^{9-}$ as shown by NMR data. Heteropoly compounds precipitated as tetrabutylammonium (TBA) or cesium salts were characterized using IR spectroscopy, differential dissolution (DD), and elemental analysis. It was found that the composition of a compound was affected not only by formation conditions in the solution, but also by the precipitant cation. In the absence of Pd(II), TBA^+ precipitated a salt of PMo_{11} heteropoly anion (HPA); Cs^+ precipitated a salt of PMo_9 HPA from the same solutions. DD analysis identified the Cs salts precipitated in the presence of Pd(II) as complexes PMo_9 and PMo_9Pd. The conclusion was drawn that Pd(II) interacted with unsaturated heteropoly molybdates more weakly than with their analogues $PW_{11}O_{39}^{7-}$ and $PW_9O_{34}^{9-}$. This weak interaction can consist in the adsorption of Pd(II) species on negatively charged HPAs.

STUDY OF THE EQUILIBRIUM OF FORMATION OF ARSENIC(III) LACUNAR HETEROPOLYTUNGSTATES BY RAMAN SPECTROSCOPY

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Russ. Chem. Bull., 52(2) (2003) pp. 370–374.

The formation of lacunar heteropolyanions (HPA): $[AsW_9O_{33}]^{9-}$, $[As_2W_{19}O_{67}(H_2O)]^{14-}$, and $[As_2W_{20}O_{68}(H_2O)]^{10-}$ in aqueous solutions was investigated by Raman spectroscopy at $[Na_2HAsO_3]_0 = 0.1$, $[Na_2WO_4]_0 = 0.9$ mol L^{-1} and pH 9.4–1.6. The $[AsW_9O_{33}]^{9-}$ HPA is characterized by the most intense band ν_s (W=O) at 948 cm^{-1} retaining its position in the pH range from 8.9 to 7.5. Under these conditions, the equilibrium constant of $[AsW_9O_{33}]^{9-}$ formation from $H_2AsO_3^-$ and WO_4^{2-} ions was estimated (log K = 87.0±1.0). The asymmetrical band at 952 cm^{-1} corresponding to $H_x[As_2W_{19}O_{67}(H_2O)]^{(14-x)-}$ shifts to 960 cm^{-1} as the pH decreases from 6.5 to 5.5, which is due to the change in HPA protonation. The $[As_2W_{20}O_{68}(H_2O)]^{10-}$ HPA is formed at pH 3.1–1.6; it is characterized by a band at 972 cm^{-1}.

THERMAL TRANSFORMATIONS OF α-$H_6P_2Mo_{18}O_{62}\cdot nH_2O$ HETEROPOLYACID

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Russ. Chem. Bull.,
52(1) (2003) pp. 103–108.

According to the ^{31}P NMR spectroscopy, heteropolyacid (HPA) $H_6P_2Mo_{18}O_{62}\cdot nH_2O$ (P_2Mo_{18}), α-isomer of the Dawson structure, transforms upon heating above 80°C partially (up to 30%) to γ-isomer, in which both polar groups Mo_3O_{13} of the heteropolyanion are turned by 60° around the X_3 axis, and partially to β-isomer in which only one group is turned. The β- and γ-isomers of P_2Mo_{18} have been found for the first time. Their transformation into the α-isomer occurs upon rehydration in one week in air and in 1 h in an aqueous solution. HPA P_2Mo_{18} decomposes on heating up to 350 °C to HPA $H_3PMo_{12}O_{40}$ (PMo_{12}) and a previously unknown phase of the $HPMo_6P_{21}$ composition, which in its turn decomposes at ~375 °C to molybdenyl phosphates and MoP_3. The PMo_{12} decomposition occurs via two routes to form the same products at temperatures of ~400 and 450 °C with corresponding exotherms of MoP_3 crystallization.

THE STRUCTURE OF NEW HETEROMETALLIC Ru/M (M = Cu, Ni, Co, Zn) COMPLEXES INVESTIGATED BY COMBINED SPECTROSCOPIC AND MODELING STUDIES

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J. Mol. Struct.,
611(1–3) (2002) pp. 131–138.

This article concerns new heterometallic Ru/M (M=Cu, Ni, Co, Zn) complexes formed upon solvent extraction of $[RuNO(NO_2)_4OH]^{2-}$ by trioctylphosphine oxide or calix[4]arene-tetraphosphine oxide. They have been characterised by IR, UV, EXAFS, and mass spectroscopies in hexane and dichloroethane solutions and by quantum mechanics calculations (PM3-tm, DFT B3LYP) in the gas phase. In these complexes, Ru and M are connected by OH and NO_2 bridging groups.

THE EXTRACTION OF HETEROMETAL COMPLEXES OF RUTHENIUM(II) WITH TRIOCTYLPHOSPHINE OXIDE FROM NITRATE SOLUTIONS

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Russ. J. Inorg. Chem.,
48(6) (2003) pp. 923–930.

Synergic extraction of $[RuNO(NO_2)_4OH]^{2-}$ with trioctylphosphine oxide in the presence of nonferrous metals (M) is studied. The extraction is due to the formation of heterometal Ru/M complexes in which M^{2+} is coordinated to ruthenium via OH and NO_2 oxygens and the extractant is coordinated to M^{2+}. The complexes have a tetrahedral or octahedral configuration. The extraction constants of these complexes have the order (Zn^{2+}–Cu^{2+}–Co^{2+}–Ni^{2+}) that follows the Irving–Williams stability row.

THE EFFECT OF NONFERROUS METALS ON THE EXTRACTION OF RUTHENIUM(II) NITROSONITRO SPECIES FROM NITRATE SOLUTIONS WITH TRIBUTYL PHOSPHATE

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Russ. J. Inorg. Chem.,
48(7) (2003) pp. 1107–1113.

An NMR study of differently charged ruthenium(II) nitrosonitro species in solutions was performed, and their reactivity to nonferrous metals was examined in the course of extraction with tributyl phosphate (TBP). A strong synergetic effect due to the formation of heterometallic Ru–M complexes was found for the most stable $[RuNO(NO_2)_4OH]^{2-}$ species. The stoichiometry and extraction constants of these complexes were determined; their extraction constants agree with the Irving–Williams series ($Cu^{2+} \geq Zn^{2+} > Co^{2+} > Ni^{2+}$).

KINETICS OF THE OXIDATION OF REDUCED Mo-V-PHOSPHORIC HETEROPOLY ACID SPECIES WITH DIOXYGEN IN CONCENTRATED AQUEOUS SOLUTIONS

E.G. Zhizhina, V.F. Odyakov, M.V. Simonova, K.I. Matveev

React. Kinet. Catal. Lett.,
78(2) (2003) pp. 373–379.

Concentrated (0.2 M) aqueous solutions of HP-acids, such as $H_{3+x+m}PV^{IV}_{m}V^{V}_{x-m}Mo_{12-x}O_{40}$ and their analogues with an excess VO^{2+} cation, are oxidized by dioxygen at 343 K and atmospheric pressure through intermediate active complexes (IAC) $[H_{x+m-1}PV^{IV}_{m}V^{V}_{x-m}Mo_{12-x}O_{40}{}^{4-}]\cdot[VO^{2+}]_{y}\cdot O_2$, where $m + y \geq 3$. The electron transfer to the coordinated O_2 molecule inside AC is the limiting stage at high **m**. At low **m**, the formation of IAC becomes the limiting stage that results in a sharp decrease in the oxidation rate.

KINETICS OF OXIDATION OF BUTENE-1 TO BUTANONE IN AQUEOUS SOLUTION IN THE PRESENCE OF IONS Pd^{2+} AND Mo-V-PHOSPHORIC HETEROPOLY ACID

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React. Kinet. Catal. Lett.,
80(1) (2003) pp. 171–179.

Oxidation of butene-1 to butanone in the presence of homogeneous catalysts ($PdSO_4$ + HPA-x), where HPA-x = $H_{3+x}PV_{x}Mo_{12-x}O_{40}$, $1 \leq \mathbf{x} \leq 4$, was investigated. This reaction is found to be of the 1st order with respect to C_4H_8, and of the 0.64th order with respect to Pd. The reaction rate does not depend on the HPA-x concentration and pH of the solution. The activation energy of the reaction is variable. A kinetic expression of the reaction is obtained for 303-343 K.

OXIDATION OF HYDROCARBONS BY DIOXYGEN REDUCTIVELY ACTIVATED ON PLATINUM AND HETEROPOLY COMPOUNDS

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J. Mol. Catal. A: Chem.,
204-205(1) (2003) pp. 591–597.

Based on Pt and heteropoly compounds (HPC), catalysts are applied to oxygenation of hydrocarbon substrates S (S=cyclohexane, cyclohexene, and α-pinene) in liquid phase with a mixture of O_2 and H_2 gases. Activity of the catalytic systems and composition of the oxygenated products are controlled by the nature of active intermediates generated under the action of the different HPC.

Based on Pt and heteropoly compounds (HPC), catalysts are applied to liquid-phase oxidation of cyclohexane and cyclohexene with a mixture of O_2 and H_2 gases. Platinum catalyst in the presence of PW_{11} and $PW_{11}Fe$ HPC represent the most active catalytic systems for alkene oxidation, whereas highest reactivity of cyclohexane was exhibited in the presence of PMo_{12} HPC.

Activity of the catalytic systems and composition of the oxygenated products are controlled by the nature of active intermediates generated under the action of the different HPC.

OXIDATION OF CYCLOHEXENE AND α-PINENE WITH O_2-H_2 MIXTURE IN THE PRESENCE OF SUPPORTED PLATINUM OR PALLADIUM CATALYSTS

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Russ. Chem. Bull.,
52(7) (2003) pp. 1544–1551.

Oxidation of cyclohexene and α-pinene with O_2-H_2 mixture in the catalytic systems containing Pt or Pd and heteropoly compounds (HPC) was studied. The main oxidation products are epoxides, allyl alcohols, and ketones. The highest yield of the oxidation products was obtained in the presence of the platinum catalyst in combination with HPC PW_{11} or $PW_{11}Fe$. The reaction mechanism was proposed. A relationship between the HPC composition and the nature of intermediates involved in oxidation was examined.

REDUCTIVE ACTIVATION OF DIOXYGEN IN CATALYTIC SYSTEMS INCLUDING PLATINUM AND HETEROPOLY COMPOUNDS: OXIDATION OF CYCLOHEXANE

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Catal. Lett., 84(3) (2002) pp. 163–168.

Catalytic action of the system based on platinum and heteropoly compound (HPC) was studied in the oxidation of cyclohexane with O_2H_2 gases to produce cyclohexanol and cyclohexanone. The active composition was represented by a solid bi-component catalyst prepared from the $[Pt(NH_3)_4][H_2PMo_{12}O_{40}]_2 \cdot 7H_2O$ complex salt through calcination and redox treatments. The bi-component catalysts were characterized by HREM, XPS, and IR spectroscopy. The active samples consisted of undestroyed crystalline HPC with finely dispersed Pt species, which contained both metallic and ionic states. Reversible Mo^{6+}/Mo^{5+} electron transfer in HPC was easily realized under conditions of catalytic reaction. Based on the state of the active catalysts, a scheme of O_2/H_2 activation and cyclohexane oxidation was suggested. According to the scheme, oxidation proceeded via radical hydroxyl intermediate.

HYDROXYLATION OF BENZENE BY O_2 AND H_2 GAS MIXTURE ON CATALYSTS CONTAINING PLATINUM METALS AND HETEROPOLYCOMPOUNDS

N.I. Kuznetsova, L.I. Kuznetsova, V.A. Likholobov

Catal. Ind., 4 (2003) pp. 17–23.

Gas-phase hydroxylation of benzene with a mixture of O_2 and H_2 proceeds on bi-component silica supported catalysts consisted of platinum metals and heteropoly compounds. Productivity of the catalysts referred to metal loading is considered in connection with a nature of platinum metals and heteropoly compounds, the active components loading, surface area of the silica supports and temperature of the process. The catalysts of optimal composition at appropriate temperature produce up to 400 mol of phenol per 1 g-atom of Pd or Pt per 1 hour. Activity of the catalysts is associated with zones of contact between platinum metal and heteropoly compound, which are presented in TEM image.

EPOXIDATION OF CYCLOOLEFINS WITH HYDROGEN PEROXIDE IN THE PRESENCE OF HETEROPOLY ACIDS COMBINED WITH PHASE TRANSFER CATALYST

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Russ. Chem. Bull., 52(2) (2003) pp. 480–486.

Oxidation of cycloolefins (cyclohexene, cyclooctene, and cyclododecene) with a 30% solution of hydrogen peroxide at 65°C in the presence of heteropoly acids (HPA) $H_3PW_{12-x}Mo_xO_{40}$ (x = 0-12), which are precursors of active peroxo complexes, and phase transfer catalysts Q^+Cl^-, where Q^+ is the quaternary ammonium cation containing C_4–C_{18} alkyl groups or $[C_5H_5NC_{16}H_{33}]^+$, was studied. The catalytic activity decreases in the HPA series: $H_3PW_{12}O_{40} > H_3PW_9Mo_3O_{40} > H_3PW_6Mo_6O_{40} > H_3PW_3Mo_9O_{40} > H_3PMo_{12}O_{40}$. The state of the $H_3PW_{12}O_{40}$–H_2O_2 system was studied using UV, IR, and ^{31}P NMR spectroscopies with variation of the $[H_2O_2] : [HPA]$ ratio from 2 to 200 during cyclohexene epoxidation. Despite different catalytic precursors, the reaction proceeds through the same peroxo complex.

ESTERIFICATION OF *N*-BUTANOL WITH ACETIC ACID IN THE PRESENCE OF $H_3PW_{12}O_{40}$ SUPPORTED ON MESOPOROUS CARBON MATERIALS

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Kinet. Catal., 44(6) (2003) pp. 778–787.

The adsorption of $H_3PW_{12}O_{40}$ (HPA) from methanol solutions on mesoporous carbon supports (multiwall carbon nanotubes (CFC-3) and CFC modified with nitrogen atoms (N-CFC)) was studied. It was found that up to 10 wt % HPA was irreversibly adsorbed on the surface of CFC. This character of adsorption is indicative of the strong interaction of the adsorbate (HPA molecules) with coal surface groups (carboxylic, lactone, etc.) to form intermolecular hydrogen bonds with π-electron interactions. It was found that N-containing surface centers affected the adsorption of HPA on N-CFC. The acid and catalytic properties of HPA/CFC systems in the esterification reaction of *n*-butanol with acetic acid were studied ([BuOH]/[HOAc] = 1:15 mol/mol; 80 °C). It was found that the strength of proton centers, which was determined as proton affinity, decreased upon supporting HPA. The HPA/CFC-3 systems most actively catalyzed the reaction. The catalytic activity of HPA/N-CFC depended on the nature of N-containing groups at the support surface, and it decreased with concentration of pyridine-like structures.

TWO-DIMENSIONAL NICKEL AND PALLADIUM NANOCLUSTERS SOLUBLE IN LOW-POLARITY APROTIC MEDIA

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Mendeleev Commun., 13(1) (2003) pp. 1–2.

The disk-like title nanoclusters (30–100) × (15–20) Å in size were prepared by the reduction of polynuclear Ni^{II} and Pd^{II} trimethylacetato complexes with BuLi, Et_3Al or $Bu^i{}_3Al$ and characterized using TEM, SAXS and EXAFS.

Photocatalytic and Related Processes

EFFECT OF THE ACIDITY OF TiO_2 SURFACE ON ITS PHOTOCATALYTIC ACTIVITY IN ACETONE GAS-PHASE OXIDATION

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Catal. Lett., 86(4) (2003) pp. 169–172.

The effect of the surface acidity of modified TiO_2 samples on the rate of photocatalytic decomposition of acetone vapor was studied. The TiO_2 activity was shown to depend strongly on the concentration of acid and basic sites on the surface. It was 1.23 times greater for TiO_2 treated with 10 M H_2SO_4 solution than for the untreated sample. This dependence may be related to changes in the adsorption energy of the reagents.

KINETICS OF THE TiO_2 FILMS GROWTH AT THE HYDROTHERMAL HYDROLYSIS OF $TiOSO_4$

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React. Kinet. Catal. Lett., 79(1) (2003) pp. 77–84.

Thin TiO_2 films were produced on different supports (quartz, silicon, plexiglas plates, stainless steel mesh) by controlled hydrolysis of $TiOSO_4$ at 80 °C. The influence of $TiOSO_4$ concentration in the range of 0.003–0.04 M and concentration of H_2SO_4 in the range of 0.002–0.04 M on the kinetics of the TiO_2 film growth was investigated. It was found that typical kinetics of TiO_2 film growth follows the sigma type and the delay time T_{ind} depends on the reagent concentrations. The existence of induction period could result from the process of nucleation of hydrated titanium oxide molecules with formation of heterogeneous colloidal metatitanic acid $TiO_2{\cdot}xH_2O$. Analysis of the kinetics was performed including the autocatalytic stage of colloidal metatitanic acid formation.

INFLUENCE OF HUMIDITY AND ACIDITY OF THE TITANIUM DIOXIDE SURFACE ON THE KINETICS OF PHOTOCATALYTIC OXIDATION OF VOLATILE ORGANIC COMPOUNDS

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Russ. Chem. Bull., 52(5) (2003) pp. 1100–1105.

The influence of the humidity and acidity of the TiO_2 surface on the kinetics of the photocatalytic processes of deep oxidation of volatile organic compounds was studied. At ~20 °C the rates of acetone and benzene oxidation are maximum at the coverages of TiO_2 with water close to monolayer and are 3-5 times higher than that in the dry atmosphere. The activation energy of benzene oxidation ($Ea = 6.3\pm0.4$ and 43.0 ± 3.2 kJ mol^{-1} at relative humidities of 8 and 70 %, respectively) at a humidity higher than 30 % decreases according to the exponential law with an increase in the surface acidity when multilayer water films are formed on the surface. Under the real conditions of operation of photocatalytic air purifiers, a TiO_2 particle is covered by water nanofilms. As in aqueous solutions, photoprocesses on the TiO_2 surface depend substantially on the solvation of the participants of the reaction, the formation of the double electric layer, and the concentration of the electrolyte (due to the dissociation of the surface acid-base groups).

GAS-PHASE PHOTOCATALYTIC OXIDATION OF DIETHYL SULFIDE OVER TiO_2: KINETIC INVESTIGATIONS AND CATALYST DEACTIVATION

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Appl. Catal., B, 42(1) (2003) pp. 77–87.

The gas-phase heterogeneous photocatalytic oxidation of diethyl sulfide (DES), a simulant for chemical agent mustard gas, was investigated in a batch reactor using detection of gaseous products and FT-IR identification of surface species. Acetaldehyde and ethylene were detected as gaseous intermediates and diethylsulfone and carboxylates were detected as surface intermediate products. It was found that DES is oxidized completely and the final products of its oxidation are carbon dioxide, water and surface sulfate species. Deactivation of the TiO_2 photocatalyst was evidenced by increased time of DES complete mineralization in consecutive treatment of fixed amount of DES in the batch reactor. Carbonate and sulfate species were detected on the TiO_2 surface after complete DES oxidation by means of FT-IR diffuse reflectance spectroscopy. These structures turned out to be responsible for TiO_2 deactivation.

TiO_2 REACTIVATION IN PHOTOCATALYTIC DESTRUCTION OF GASEOUS DIETHYL SULFIDE IN A COIL REACTOR

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Appl. Catal., B, 44(1) (2003) pp. 25–40.

Diethyl sulfide (DES) photocatalytic oxidation was carried out in a flow research reactor with TiO_2 Hombikat UV 100 deposited onto the internal surface of a Pyrex coil. The reactor allowed easy catalyst reactivation by washing with water. Mass transfer limitations were not detected in the reactor. Catalyst deactivated after several hours of complete DES mineralization, which was expressed by decrease of effluent CO_2 concentration and appearance of gaseous intermediates. Catalyst reactivation was achieved by two procedures: (1) irradiating photocatalyst until complete mineralization of adsorbed organic products with subsequent water washing; and (2) immediate washing with water. The water used after the first procedure contained only H_2SO_4, while after the second procedure it contained organic intermediates. The second procedure was much faster. Lower water concentration and higher catalyst loading allowed longer catalyst stability in DES oxidation. Low feed DES concentration resulted in much longer deactivation. Twelve consecutive runs were done to test reactivation completeness. Some permanent catalyst deactivation was noted and explained by TiO_2 etching with H_2SO_4. Gaseous and surface intermediate products were detected in the reactor effluent and catalyst wash water using solid phase microextraction (SPME) and trimethylsilyl derivatization. Main gaseous products were acetaldehyde, diethyl disulfide, ethylene, SO_2, and main surface products were diethyl disulfide, diethyl trisulfide, 1,2-bis(ethylthio)ethane, ethanesulfinic, ethanesulfonic acids, diethyl sulfoxide, diethyl sulfone, and sulfuric acid.

PHOTOCATALYTIC DEGRADATION OF 2-PHENETHYL-2-CHLOROETHYLSULFIDE IN LIQUID AND GAS PHASES

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Environ. Sci. Techn., 36(23) (2002) pp. 5261–5269.

This work explores the ability of photocatalysis to decontaminate water and air from chemical warfare agent mustard using its simulant 2-phenethyl 2-chloroethyl sulfide (PECES). PECES like mustard slowly dissolves in water with hydrolysis, forming 2-phenethyl 2-hydroxyethyl sulfide (PEHES). Irradiation of TiO_2 suspension containing PECES with the unfiltered light of a mercury lamp ($\lambda \geq 254$ nm) decomposed all PECES mostly via photolysis. Reaction under filtered light ($\lambda > 300$ nm) proceeds mainly photocatalytically and require's longer time. Sulfur from starting PECES is completely transformed into sulfuric acid at the end of the reaction. Detected volatile, nonvolatile, surface products, and the suggested scheme of degradation are reported. The main volatile products are styrene and benzaldehyde, nonvolatile – hydroxylated PEHES, surface 2-phenethyl disulfide. Photolysis of PECES produced the same set of volatile products as photocatalysis. Photocatalytic degradation of gaseous PECES in air results in its mineralization but is accompanied by TiO_2 deactivation. The highest rate of mineralization with minimum deactivation was observed at about room temperature and a water concentration of 27 500 ppm. No gaseous products except CO_2 were detected. The main extracted surface product was styrene. It was concluded that PECES photocatalytic degradation proceeds mainly via C-S bond cleavage and further oxidation of the products. Hydrolysis of the C-S bond was detected only in gas-phase photocatalytic degradation. The quantum efficiency of gas-phase degradation (0.28 %) was much higher than that of liquid-phase degradation (0.008 %). The results demonstrate the ability of photocatalysis to decontaminate an aqueous and especially an air environment.

THE ROLE OF PLATINUM DEPOSITED ON TiO_2 IN PHENOL PHOTOCATALYTIC OXIDATION

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Langmuir, 19(8) (2003) pp. 3151–3156.

Photooxidation of phenol has been studied in aqueous suspensions of titanium dioxide Hombikat UV100 and Degussa P25 loaded with various amounts of Pt. The rates of phenol decomposition and total carbon removal rose by a maximum factor of 1.5 when Hombikat was loaded with 1 wt % Pt; further increase of Pt deposition did not increase the photoactivity any more. The electron movement across the Pt-anatase junction is discussed, and the positive influence of Pt on phenol oxidation over Hombikat is explained by the increase of charge separation in agglomerates of primary particles. The photocatalytic activity of P25 was higher than that of platinized and pure Hombikat. But loading P25 with Pt resulted in a decrease of phenol decomposition and total carbon removal rates. The decrease of Degussa P25 activity after platinization means that Pt cannot further increase the efficiency of charge separation in this TiO_2, whose two-phase composition already provides a very efficient suppression of recombination in liquid photocatalytic reaction. The charge separation in P25 is illustrated with the scheme of P25's band structure. The possible side effects brought by Pt deposition are also discussed.

ENHANCED PHOTOCATALYTIC DEGRADATION OF DIMETHYL METHYLPHOSPHONATE IN THE PRESENCE OF LOW-FREQUENCY ULTRASOUND

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Photochem. Photobiol. Sci.,
2(6) (2003) pp. 694–698.

Mechanistic aspects of the role of 20 kHz ultrasonication in photocatalytic oxidation of dimethyl methylphosphonate (DMMP), a simulant for nerve chemical warfare agents, were studied in a batch reactor. It was found that DMMP did not undergo mineralization under low frequency (20 kHz) ultrasonic irradiation. The increase of the rate of DMMP photocatalytic mineralization in the presence of ultrasound was not due to deagglomeration of TiO_2, but was associated with enhanced mass transport of reagents. The same intermediate non-volatile products were detected in photocatalytic and sonophotocatalytic degradation. A kinetic model involving all stable intermediate species detected was introduced. Apparent rate constants of all stages of DMMP mineralization increase under sonication. A reaction route of DMMP mineralization without the formation of intermediate products appeared under ultrasonication. Such behaviour was attributed to enabling mass transport of DMMP into micropores and to the surface of TiO_2.

HETEROGENEOUS OXIDATION OF ETHANOL OVER $Cu(OH)_2/\alpha\text{-}Fe_2O_3$ UNDER VISIBLE LIGHT

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React. Kinet. Catal. Lett.,
78(2) (2003) pp. 341–348.

A $Cu(OH)_2/\alpha\text{-}Fe_2O_3$ photocatalyst is shown to be active in the gas phase oxidation of ethanol under visible light. The calculated initial quantum efficiency of the ethanol photooxidation is 0.1-1 %. However, ethanol is oxidized only into acetic acid, which deactivates the catalyst.

Electrocatalysis and Electrochemical Processes

CO-ADSORPTION OF FLUORIDE AND HYDROXIDE IONS ON Ag(111) IN ALKALINE ELECTROLYTES: ELECTROCHEMICAL AND SHG STUDIES

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Z. Phys. Chem, 217(5) (2003) pp. 557–572.

Hydroxide (OH^-) adsorption at Ag(111)/alkaline electrolyte interfaces is the initial step leading to the formation of surface oxide. It is investigated how OH^- anion adsorption is influenced by co-adsorption of supporting electrolyte anions (F^-). Pure NaF and NaOH as well as mixed electrolytes ranging from pH = 5.8 to 14 are investigated. The rotational anisotropy of the second harmonic generation (SHG) signal is measured to distinguish adsorptive processes from structural changes on the Ag surface. The results obtained clearly show a cross-over from F^--dominated to OH^--dominated adsorption, while both species remain charged upon adsorption. At more positive potentials, but below the reversible potential of bulk oxide growth, OH is discharged leading to sub-monolayer oxide build-up, whereas in acidic electrolyte, Ag is dissolved. At intermediate pH, the formation of a structured OH^-/F^- co-adsorbed layer is proposed.

ELECTROCHEMICAL SHG AT A Ag (111) SINGLE-CRYSTAL ELECTRODE USING THE HANGING MENISCUS CONFIGURATION

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Appl. Phys. B, 74(7-8) (2002) pp. 635–639.

In situ electrochemical second-harmonic generation (SHG) were combined with voltammetry measurements using the hanging meniscus configuration. This setup is used to investigate the interface between a Ag (111) electrode and an alkaline electrolyte. The study offers a new *in situ* insight into the electrochemical processes at the Ag (111) electrode during OH adsorption and subsequent oxidation. The behavior of SHG isotropic and anisotropic contributions as a function of potential is discussed and related to the interfacial electric field. Comparison of the results with previous investigations of the Ag underpotential oxidation in alkaline solutions shows that submonolayer oxidation is followed by bulk oxidation.

STRUCTURE AND DYNAMICS OF THE INTERFACE BETWEEN A Ag SINGLE CRYSTAL ELECTRODE AND AN AQUEOUS ELECTROLYTE

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Faraday Discuss., 121 (2002) pp. 181–198.

The aim of this work is to elucidate the initial steps of the electrochemical oxidation of Ag(111) in alkaline electrolytes. Electrochemical as well as *ex situ* (XPS) and *in situ* (SHG) spectroscopic techniques was used to reconstruct the Ag(111)/electrolyte interface as a complex dynamic entity. Moving in the direction from negative to positive potentials it was observed for the first time specific adsorption of hydroxide ions, which starts at *ca.* –1.1 V *vs.* Ag/Ag_2O in 0.1 M NaOH. SHG data prove that hydroxide retains its negative charge. At -0.3 V oxidation of the surface sets in with the formation of negatively charged adsorbed oxygen species and Ag^+ ions, which give rise to peaks at 528.2 ± 0.2 eV and at 367.7 eV in the O 1s and the Ag $3d_{5/2}$ XP spectra, respectively. Around –0.1 V the adlayer is transformed into an ordered surface oxide phase which grows *via* a nucleation and growth mechanism. Above the reversible Ag/Ag_2O potential the 2D Ag(I) oxide transforms into a 3D Ag(I) oxide. The electrochemical oxidation is compared with the previously studied gas-phase process, demonstrating both remarkable similarities as well as some differences.

MODEL APPROACH TO EVALUATE PARTICLE SIZE EFFECTS IN ELECTROCATALYSIS: PREPARATION AND PROPERTIES OF Pt NANOPARTICLES SUPPORTED ON GC AND HOPG

O.V. Cherstiouk, P.A. Simonov, E.R. Savinova

Electrochim. Acta,
48(25-26) (2003) pp. 3851–3860.

Although metal nanoparticles are widely used in electrocatalysis, in particular for the preparation of the electrodes for fuel cells, it is still not fully understood how the size of a metal phase affects its electrochemical reactivity. In this paper, a possible approach to design model electrodes for studying size effects in electrocatalysis is demonstrated. A simple chemical deposition procedure is introduced, which allows reproducible preparation of 1.5/3.0 nm Pt nanoparticles anchored to the surface of glassy carbon (GC) or highly oriented pyrolytic graphite (HOPG). Pt nanoparticles supported on GC are stable versus potential variation and can be used for studying size effects. They are examined in electrochemical reactions relevant to low-temperature fuel cells: electrooxidation of adsorbed CO and methanol. It is demonstrated that reactivity of Pt nanoparticles in these reactions is considerably decreased in comparison to bulk polycrystalline Pt.

CO MONOLAYER OXIDATION AT Pt NANOPARTICLES SUPPORTED ON GLASSY CARBON ELECTRODES

O.V. Cherstiouk, P.A. Simonov, V.I. Zaikovskii, E.R. Savinova

J. Electroanal. Chem., 554-555 (2003) pp. 241–251.

CO monolayer oxidation on glassy carbon supported 1–2 nm Pt nanoparticles is studied using potential sweep and potential step methods. The CO stripping peak on the nanoparticles is significantly shifted to positive potentials vs. the corresponding feature at bulk polycrystalline Pt. Current transients at nanoparticulate electrodes are highly asymmetric with a steep rise, maximum at $\theta_{CO}\approx0.8–0.9$, and a slow decay following $t^{-1/2}$. The experimental results are compared to the theoretical models of adsorbed CO oxidation described in the literature. A tentative model is suggested to account for the experimental observations, which comprises spatially confined formation of oxygen containing species at active sites, and slow diffusion of CO molecules to the active sites, where they are oxidized. The upper limit of the CO surface diffusion coefficient at Pt nanoparticles is estimated as approximately 4×10^{-15} cm^2 s^{-1}.

DISPERSE ELECTROLYTIC PLATINUM AND PALLADIUM DEPOSITS OF SUBMICRON THICKNESS ON POLYCRYSTALLINE SUPPORTS: AN X-RAY DIFFRACTOMETRY AND MICROSCOPY STUDY

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Russ. J. Electrochem., 38(10) (2002) pp. 1116–1132.

The structure of model electrode materials broadly used in electrocatalysis (platinized platinum, palladized platinum, platinized gold) is studied by X-Ray diffractometry, scanning electron microscopy, and transmission electron microscopy. Disperse platinum and palladium coatings less than 1 μm thick are obtained by potentiostatic or galvanostatic deposition from solutions of complex chloride salts. Lattice parameters of disperse metals are shown to be considerably smaller than those of bulky crystals. Some new tendencies of variations in structural parameters with the deposition potential are revealed. Special attention is paid to a reliable determination of the size of regions of coherent scattering (ROCS) and microdistortion; in connection with this, results of approximation of reflections by various functions and a harmonic analysis of reflections are compared. The latter are used for constructing ROCS distributions by size. Good agreement is found with the STM data for platinum deposits obtained earlier. Conversely, in the case of palladium deposits, ROCS are smaller than the particle size in an outer layer of the deposit by the STM data. This result is interpreted in terms of strong concrescence of palladium nanoparticles. To determine the true surface areas of deposits and estimate continuousness of covering the support by the deposit and regularities of platinum aging on gold in conditions of potential cycling, a voltammetry method is applied.

KINETICS OF ELECTROCHEMICAL REACTIONS: FROM SINGLE CRYSTALS TO nm-SIZED SUPPORTED PARTICLES

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Surf. Sci., 521(1-2) (2002) L655–L661.

The rate of electrochemical reactions including electron transfer is influenced by the electric field near the electrode(s). Scrutinizing this effect, it has been shown that the dependence of the electric field near the flat single-crystal electrode on adsorbate coverage may result in increase (up to one order of magnitude) of a rate constant of electrochemical reaction with increasing coverage. In addition, it was demonstrated that due to specific distribution of the electric field the rate of electrochemical reaction occurring on supported nm-sized metal particles may be higher (by a factor of 5) than on the flat surface. Finally, the implications of these findings for interpretation of experimental data are briefly discussed.

SIMULATION OF CO ELECTROOXIDATION ON nm-SIZED SUPPORTED Pt PARTICLES: STRIPPING VOLTAMMETRY

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Chem. Phys. Lett., 376(1-2) (2003) pp. 220–225.

The kinetics of CO electrooxidation on nm-sized supported Pt crystallites exhibiting (111) and (100) facets is analyzed. Specifically, it has been shown how the CO-diffusion-mediated communication between these facets may modify voltammograms observed by using CO stripping voltammetry. The results obtained demonstrate that the reaction kinetics for nm-sized particles can be remarkably different compared to those expected on the basis of simple superposition of the kinetics corresponding to the infinite faces. These findings have implications for interpretation of experimental data and for the design of real catalysts and also have important consequences for the efforts to bridge the so-called structure gaps in electrocatalysis.

REPLY TO COMMENT ON: "nm-SIZED METAL PARTICLES ON A SEMICONDUCTOR SURFACE, SCHOTTKY MODEL, ETC."

V.P. Zhdanov

Surf. Sci., 530(3) (2003) pp. 219–220.

The available estimates of the charge transferred from a semiconductor to supported nm-sized metal particles are based on the models constructed in analogy with the Schottky model describing the interface between a bulk metal and semiconductor. In this brief discussion, it is articulated that such models appreciably overestimate the transferred charge.

ELECTROCHEMICAL REACTIONS ON CATALYST PARTICLES WITH THREE-PHASE BOUNDARIES

V.P. Zhdanov

Phys. Rev. E, 67(4) (2003) 042601 (4 pp.).

In fuel cells, electrochemical reactions are often assumed to occur on metal catalyst particles contacting simultaneously the ion-conducting electrolyte and gas phase. Monte Carlo simulations demonstrate that in this case the deviations from the Tafel law in the dependence of the reaction rate on the electrode potential may be related to diffusion of one of the adsorbed reactants along catalyst particles.

PROTON CONDUCTIVITY IN $H_3OFe(SO_4)_2$-SiO_2 COMPOSITES

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Russ. J. Inorg. Chem., 48(7) (2003) pp. 955–960.

Proton composite electrolytes of composition $(1-x)H_3OFe(SO_4)_2 \cdot xSiO_2$ ($x = 0.1$–0.6) have been prepared. Ultrafine silica increases the proton conductivity of the hydrogen sulfate by one to two orders of magnitude. The conductivity of the composites is a significant function of composition and peaks at x=0.3 for samples heated at 380 or 440 K. In the highest conductivity composites prepared at 440 K, the starting acid salt changes its composition.

Biotechnology and Biology Related Catalysis

BIOEPOXIDATION OF PROPYLENE BY NON-GROWING CELLS OF *RHODOCOCCUS* SP.

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Chem. Sustain. Devel.,
11(1) (2003) pp. 117–122.

The biotechnological potential of *Rhodococcus* sp. bacteria for direct selective bioepoxidation of propylene to propylene oxide has been investigated. The kinetics of accumulation of propylene oxide in suspensions of the non-growing bacterial cells has been studied. The effect of propylene oxide produced on biocatalytic activity of *Rhodococcus* cells has been investigated. The study of bacteria adsorption on various carbon-containing inorganic supports has been started to develop efficient adsorbents for *Rhodococcus* immobilization.

NON-GROWING RHODOCOCCUS SP. CELLS AS SELECTIVE CATALYSTS OF DIRECT OXIDATION OF PROPYLENE INTO PROPYLENE OXIDE

G.A. Kovalenko, E.V. Kuznetsova

Catal. Ind., 5 (2003) 37–43.

Rhodococcus ruber propane-assimilating microorganisms (the city of Perm) are shown to carry out the process of direct propylene bioepoxidation with initial velocity of 110 nmole/mg of dry cells. The reaction product is propylene oxide, it irreversibly inhibits monooxygenase activity of non-growing rhodococcus bacterial cells. Diverse mineral, carbon, and carbon-mineral carriers have been prepared and investigated to carry out the process in the heterogeneous conditions. Macrostructured ceramic carriers, on the surface of which a layer of catalytic fibrous carbon is synthesized, are optimal adsorbents for non-growing bacterial Rhodococcus sp. cells.

CARBON-CONTAINING MACROSTRUCTURED CERAMIC SUPPORTS FOR ADSORPTIVE IMMOBILIZATION OF ENZYMES AND BACTERIA.
3. BIOCATALYTIC PROPERTIES OF ADSORBED INVERTASE

G.A. Kovalenko, L.V. Perminova, O.V. Komova, A.V. Simakov, V.V. Khomov, O.Yu. Borovtsova, N.A. Rudina

Biotechnology, 4 (2003) pp. 52–62.

Systematic studies of adsorptive immobilization of invertase on macrostructured carbon-containing ceramic supports were aimed at development of highly stable heterogeneous biocatalyst for continuous process of inverted sugar production. The surface carbon layer with a loose filamentous structure formed by catalytic carbon (CFC) was shown to possess the optimal morphology for effective adsorption and stabilization of yeast invertase, whereas the immobilized enzymes were completely deactivated on smooth graphite-like carbon. Kinetic regularities of sugar inversion were studied. Michaelis-Menten constants were estimated for invertase in soluble and immobilized states. Kinetics of conversion of sucrose was studied in flow bioreactors using the prepared differently shaped biocatalysts (granules, foam ceramics, honeycomb monoliths).

INNOVATIVE BIOCATALYTIC PROCESSES FOR SWEETENERS PRODUCTION

V.N. Parmon, G.A. Kovalenko

Storage Process. Agriculture,
8 (2003) pp. 116–120.

Theoretically, the proposed innovative technologies of *heterogeneous biocatalytic processes* for sweeteners production (starch treacle and inverted sugar syrups) are rather attractive for the market and may be profitable. The expected demand is high enough both from big industrial enterprises to modernize the facilities and from venture entrepreneurs to offer products and services.

THE CATALYTIC METHOD OF VERBANOL PREPARATION WITH CONTROLLED ISOMER DISTRIBUTION STARTING FROM RENEWABLE MATERIAL α-PINENE

I.L. Simakova, V.A. Semikolenov

Chem. Sustain. Devel.,
11(1) (2003) pp. 271–275.

The reasonable scheme of commercially valuable odour chemicals syntheses starting from renewable natural material α-pinene includes the explored reaction of verbenol hydrogenation into verbanol under mild conditions over Pd/C catalyst. The possibility of verbanol stereoisomers preparation with controlled isomer distribution that defines a practical use of scheme as a whole is considered. The effects of the hydrogen pressure, temperature and catalyst content on the isomers re-proportioning in the course of verbenol hydrogenation are studied. The main factors permitting the hydrogenation process to direct to the definite verbanol isomers production were found to be hydrogen pressure and reaction temperature. Isoverbanol/neoisoverbanol ratio increases with hydrogen pressure growth from 2 to 11 bar and temperature decrease from 50 to 90 °C.

LINALOOL TO GERANIOL/NEROL ISOMERIZATION CATALYZED BY $(RO)_3VO$ COMPLEXES: STUDIES OF KINETICS AND MECHANISM

V.A. Semikolenov, I.I. Ilyna, R.I. Maksimovskaya

J. Mol. Catal. A: Chem.,
204-205(1) (2003) pp. 201–210.

Highly selective catalytic system $\{(RO)_3VO+[(Bu)_4N+]OH\}$ for the process of linalool to geraniol+nerol isomerization within the temperature range of 413–513 K is reported. Using the ^{51}V NMR spectroscopy, composition and reactivity of vanadium complexes formed in the catalytic system were investigated. Mononuclear vanadium complexes $(RO)_{3-n}(R'O)_nVO$, where RO - linalyl and R′O - geranyl/neryl ligands, n=0, 1 and 2, are active in the isomerization reaction. The reaction of the ligand {linalool/(geraniol+nerol)} exchange is very fast and reversible, the equilibrium constant of this reaction was estimated. The rate determining step of the isomerization process is the rearrangement of the coordinated to vanadium linalyl- to geranyl/neryl ligands which, probably, proceeds via reduction–oxidation mechanism. The isomerization of linalool is a reversible reaction and two isomers (geraniol and nerol) are formed by the parallel routs. The equilibrium constant of the linalool/(geraniol+nerol) as well as geraniol/nerol isomerization slightly depends on temperature. The reaction rate is of the first-order on linalool, geraniol and nerol concentrations. The kinetic scheme and mechanism of linalool to geraniol+nerol isomerization are suggested.

Sorption Properties of Composite Sorbents

EXPERIMENTAL STUDY ON THE KINETICS OF WATER VAPOR SORPTION ON SELECTIVE WATER SORBENTS, SILICA GEL AND ALUMINA UNDER TYPICAL OPERATING CONDITIONS OF SORPTION HEAT PUMPS

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Int. J. Heat Mass Transfer,
46(2) (2003) pp. 273–281.

A selective water sorbent (SWS) is a composite material consisting of a porous host matrix and a hygroscopic substance (commonly an inorganic salt) impregnated into its pores. This work presents an experimental investigation for the kinetics of water vapor sorption on two host materials; namely mesoporous silica gel and alumina in comparison with the two composites SWS-1L and SWS-1A formed by impregnating these two host matrices with $CaCl_2$. Moreover, the kinetics of water vapor sorption on microporous silica gel has been also investigated. The measurements have been carried out on 3 g samples of loose pellets on an isothermal wall under three different operating conditions of sorption heat pumps. The results obtained evidence a remarkable increase in the differential water loading of both SWS-sorbents over their host materials. However, and due to the increased diffusion resistance to water sorption resulting from the salt impregnation, the kinetics of water sorption into the host matrices is faster than that into the two SWS-composites. Moreover, SWS-1L is found to be faster than SWS-1A in sorbing water vapor. The differential water loading on microporous silica is about twice that on mesoporous silica and alumina, but the sorption kinetics are a little bit slower.

SORPTION OF WATER BY SODIUM, COPPER, AND MAGNESIUM SULFATES DISPERSED INTO MESOPORES OF SILICA GEL AND ALUMINA

L.G. Gordeeva, I.S. Glaznev, Yu.I. Aristov

Russ. J. Phys. Chem.,
77(10) (2003) pp. 1715–1720.

New composite sorbents [Na_2SO_4/(KSK silica gel), $CuSO_4$/KSK, $MgSO_4$/KSK, and $MgSO_4$/alumna] were synthesized. The sorption equilibrium of these sorbents with water vapor was studied at pressures from 10 to 50 mbar and temperatures from 20 to 300 °C. It was established that the sorption equilibrium and phase composition of Mg, Na, and Cu sulfates dispersed into pores of KSK silica gel are determined by the concentration of the salt in the composite. At low concentrations of the salt, it exists in the pores in the form of an XRD-amorphous phase, whose composition changes monotonically with the water vapor pressure and the temperature (bivariant system). In the pores of systems containing high concentrations of Mg and Na sulfates, a crystalline phase of the salt is formed. The dispersity of this phase is determined by the size of the pores in silica gel, 10–25 nm. The sorption of water vapor by these systems is accompanied by the formation of a salt crystal hydrate with a fixed composition (univariant systems). As the sorption of water vapor proceeds still further, a salt solution is formed in the pores, and the system becomes bivariant. Depending on the nature of the salt, the crystalline phase is formed at a salt concentration of 15 to 25 wt %. The characteristics of the sorption of water vapor by dispersed sulfates were compared with those reported for Ca and Li halides dispersed in the same matrices.

SORPTION PROPERTIES OF CALCIUM CHLORIDE DISPERSED IN SILICA GEL PORES

L.G. Gordeeva, I.S. Glaznev, V.V. Malakhov, Yu.I. Aristov

Russ. J. Phys. Chem., 77(11) (2003) pp. 1843–1847.

The phase composition of composite sorbents “calcium chloride in mesopores of silica gel” with different contents of the salt was studied by differential dissolution and X-Ray powder diffraction analysis. Their sorption equilibria with water vapors were studied by thermogravimetry in a temperature range from 20 to 200 °C at p = 10 to 50 mbar. It was shown that calcium chloride interacts with silica gel to form two phases in pores, namely, crystalline bulk and X-Ray amorphous surface phases. The ratio between these phases depends on the salt content of the composite; the fraction of the crystalline phase grows with an increase in the salt concentration. The sorption equilibrium between composite sorbents and water vapors was found to be sensitive to the ratio between the crystalline and X-Ray amorphous phases. It was demonstrated that vapor sorption by high-salt sorbents, in which the salt is predominantly crystalline, is accompanied by the reaction $CaCl_2 + 2H_2O \Leftrightarrow CaCl_2{\bullet}2H_2O$; the sorbed water amount in pores changes stepwise. In low-salt sorbents with an X-Ray amorphous salt phase, the composition of the condensed phase in pores changes continuously, which is typical of solutions of salts or their hydrates with a vacancy structure.

SORPTION OF CARBON DIOXIDE BY THE COMPOSITE SORBENT “POTASSIUM CARBONATE IN POROUS MATRIX”

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I.G. Danilova, E.A. Paukshtis, E.M. Moroz,
T.A. Kriger, V.V. Malakhov, Yu.I. Aristov

Russ. Chem. Bull., 52(2) (2003) pp. 359–363.

Sorption of CO_2 in the presence of water vapor by the K_2CO_3-γ-Al_2O_3 composite sorbent was studied by IR spectroscopy *in situ*, X-Ray diffraction analysis, and the differentiating dissolution method and reasons for a decrease in its dynamic capacity are given. The samples containing $K_2CO_3 \cdot 1.5H_2O$ in pores are characterized by the maximal dynamic capacity. A mechanism for CO_2 sorption was proposed, which qualitatively explains the obtained dependence of the capacity on the water content in the composite sorbent. A high dynamic capacity can be maintained by regeneration of the sorbents by water vapor at 170 °C. The capacity of the sorbents decreases during the first 10 sorption—regeneration cycles due to the formation of an inactive phase of potassium aluminum carbonate.

Purification of Gases from Toxic Admixtures

THE Cu-ZSM-5 CATALYSTS WASHCOATED ON MONOLITH FOR DIESEL VEHICLE EMISSION CONTROL

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V.A. Sazonov, N.V. Shikina, V.V. Kuznetsov,
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Chem. Sustain. Devel., 11 (1) (2003) pp. 309–319.

The composition of modified monolith zeolite catalysts containing the basic components in the washcoating layer is suggested. When the washcoating layer contains 80% zeolite, 10% TiO_2, and 10 % Al_2O_3, the catalyst exhibits both activity and adhesion strength. The titanium catalyst is stable to sulfur poisoning (H_2S) at 500 °C; a small decrease in the catalyst activity at 400 °C is no longer observed after regeneration. Introducing 4 wt. % Ce (calculated for respect to the washcoating) into the ready catalyst, one can preserve the catalyst activity and provide its stable operation in the presence of water vapor both at 400 and 500 °C. Activity of the titanium-cerium-modified monolith catalyst is stable in the presence of water vapor and sulfur compounds in the gas mixture at a time.

STUDY OF OZONE GENERATION IN THE BED OF HETEROGENEOUS CATALYSTS OF VARIOUS GEOMETRY

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Eurasian Chem.-Technol. J.,
4(4) (2002) pp. 271–276.

An urgent worldwide problem in the field of environment protection is the development of energy saving and highly efficient technologies for removal of volatile organic compounds (VOCs) from gas emissions of large volume and emitted at rather low temperatures, such as low concentrated ventilation exhausts at room temperatures. The ozone-catalytic method is of particular interest because of his suitability for solving of “cold start” problem for automotive emissions control when the system of catalytic purification is not heated to optimal operation temperature.

From the other side, the efficiency of ozone-catalytic process significantly decreases due to the parallel reaction of ozone recombination to molecular oxygen.

For this reason, the development of devices, providing direct generation of ozone in the heterogeneous catalyst bed attracts particular interest. The application of this kind of devices leads to combination of the processes of formation of highly reactive O_3 molecule and oxidation of undesirable organic admixtures.

In this paper the results on the development of the devices for the ozone generation directly in the bed of the catalysts of different geometry (spherical and honeycomb monolith) are presented. The experiments upon variation the electric signal frequency, flow rate have been carried out. It was shown, that developed device provides effective ozone generation within frequency range 500–1000 Hz and allow effectively combine the catalytic and electric properties and can be considered as the prototype for different appliance in environment protection.

MANGANESE OXIDE MONOLITH CATALYSTS MODIFIED BY Fe AND Cu FOR HIGH-TEMPERATURE AMMONIA DECOMPOSITION AND H_2S REMOVAL

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Chem. Sustain. Devel., 11(1) (2003) pp. 75–88.

Monolith sorbents/catalysts that have potential in simultaneous removal of H_2S and NH_3 from hot fuel gas were developed. Preparation methodology and composition of supported honeycomb sorbents/catalysts, based on manganese oxides modified by Fe and Cu oxides, have been optimized. Impregnated and washcoated monolith catalysts were tested in ammonia high temperature decomposition and H_2S sorption. Approaches for improving the thermal stability and catalytic activity under reaction conditions are described.

DEVELOPMENT OF PROCESSES FOR PURIFICATION OF COAL PROCESSING GASES FROM SULPHUR AND CYAN FOR THE APPLICATION IN ENERGY TECHNOLOGIES

N.N. Kundo, G.A. Faddeenkova

Chem. Sustain. Devel., 11(4) (2003) pp. 603–609.

For the efficient use of gases formed in a number of thermochemical procedures of carbon processing, it is necessary to purify them from hazardous impurities, such as H_2S, HCN, NH_3, resinous substances. To purify the gases, it is proposed to use the liquid catalytic procedure with the soluble derivatives of cobalt phthalocyanine as a catalyst. This method allows achieving the required purification extent with low expenses. The purified gases can be used to obtain electricity and heat, and also as chemical raw material for obtaining ammonia, methanol, liquid fuel, etc. Elemental sulphur is obtained as a result of purification.

Mathematical Simulation of Catalytic Processes and Reactors. Chemical Engineering

RELAXATION OSCILLATIONS IN A KINETIC MODEL OF CATALYTIC HYDROGEN OXIDATION INVOLVING A CHASE ON CANARDS

G.A. Chumakov*, N.A. Chumakova (*Sobolev Institute of Mathematics, Novosibirsk, Russia

Chem. Eng. J., 91(2–3) (2003) pp. 151–158.

A detailed study of two- and three-variable mathematical models of a heterogeneous catalytic system is presented with special attention to weakly stable dynamics, a type of complex irregular behavior frequently encountered in oscillating chemical reactions. One of the most important properties of the weakly stable dynamics is "a sensitive dependence on the initial conditions". Analysis of a global error in long-term numerical integration shows that a high sensitive dependence on the initial conditions appears in the three-variable system with fast, intermediate and slow variables due to existence of the canard cycles which occur close to Hopf bifurcation in the one-parameter family of two-variable subsystems.

WEAKLY STABLE DYNAMICS IN A THREE-DIMENSIONAL KINETIC MODEL OF CATALYTIC HYDROGEN OXIDATION

G.A. Chumakov*, N.A. Chumakova (*Sobolev Institute of Mathematics, Novosibirsk, Russia)

Chem. Sustain. Devel., 11(1) (2003) pp. 63–66.

Some new results concerning complex dynamics in a kinetic model of heterogeneous hydrogen oxidation over metallic catalysts are presented. Relaxation oscillations with a high sensitive dependence on the initial conditions arise in the three-variable system with fast, intermediate and slow variables due to existence of the canard cycles that occur in the one-parameter family of two-variable subsystems. A key feature of the weakly stable dynamics appearance will be successive period doubling bifurcations in which the system behaviour becomes progressively more complex until the attractor appears.

PARAMETRIC SENSITIVITY OF METHANOL OXIDATION PROCESS AS SOLUTION OF BOUNDARY-VALUE PROBLEM WITH AN UNKNOWN PARAMETER

N.A. Chumakova, A.I. Madyarov

Chem. Eng. J., 91(2-3) (2003) pp. 159–166.

A new approach to parametric sensitivity studies of a catalytic fixed-bed operation is presented. This approach is based on the sensitivity functions of technological characteristics with respect to small variations of control parameters under the condition that the pressure drop over the catalyst bed is fixed. The problem of parametric sensitivity of the methanol oxidation process is formulated as an example serving to illustrate the computational technique discussed in the paper. The mathematical model can be written as a boundary-value problem for ordinary differential equations with the linear gas velocity as an unknown parameter. An approach provides the possibility of estimating the influence of space-nonuniformities on the technological process characteristics in a real fixed-bed reactor using a relatively simple one-dimensional model.

INVESTIGATION OF HEAT WAVE PROPAGATION MODEL FOR AN $A_0 \rightarrow A_1 \rightarrow A_2$ CATALYTIC REACTION

E.V. Sazhenkova, N.A. Chumakova

Selçuk J. Appl. Math., 3(2) (2002) pp. 109–126.

Heat wave propagation phenomenon in heterogeneous media is a subject of big interest in the theory of unsteady-state catalytic processes in fixed bed reactors. The problem of numerical study of an one-dimensional heat wave propagation model in the case of two consequent exothermic reactions is considered. An efficient algorithm based on Godunov's orthogonal factorization method and Newton's method is described. Some recommendations are given for construction of initial approximation. In addition, influence of key physical and chemical parameters on the heat wave properties is studied.

MATHEMATICAL MODELLING OF EXOTHERMIC CATALYTIC REACTION IN A SINGLE PARTIALLY-WETTED POROUS CATALYST PARTICLE

I.A. Mikhailova, V.A. Kirillov, S.I. Fadeev*, M.G. Slinko** (*Sobolev Institute of Mathematics, Novosibirsk, Russia; **Karpov Institute of Physical Chemistry, Moscow, Russia)

Chem. Eng. J., 91(2-3) (2003) pp. 181–189.

The mathematical model for the multiphase steady-state processes on a partially-wetted porous catalyst slab in the conditions of the exothermic catalytic reaction, species diffusion, phase transitions, and capillary phenomena interaction is developed. Numerical experiment was carried out for the model reaction of α-methylstyrene hydrogenation. The impact of the external wetting efficiency on the steady-state regimes of the slab is investigated. The partially-wetted regime is characterized by studying the width of the dry zone inside the slab: the slab overheating, the area of the multiplicity.

MODELING OF CRITICAL PHENOMENA FOR LIQUID/VAPOR–GAS EXOTHERMIC REACTION ON A SINGLE CATALYST PELLET

A.B. Shigarov, A.V. Kulikov, N.A. Kuzin, V.A. Kirillov

Chem. Eng. J., 91(2-3) (2003) pp. 205–213.

Physical mechanisms are discussed and crude mathematical models with lumped parameters are developed, which explain the authors recent experimental data, concerning temperature hysteresis and multiplicity phenomena for α-methylstyrene (AMS) liquid–vapor hydrogenation on a single catalyst pellet. The interplay between endothermic vaporization and exothermic vapor phase reaction is elucidated. The results of this study may help to develop more sophisticated models and theory of hot spots formation and runaway phenomena in trickle-bed reactors.

CALCULATING THE LIQUID-GAS EQUILIBRIUM IN THE FISCHER-TROPSCH SYNTHESIS

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Theor. Found. Chem. Eng.,
37(2) (2003) pp. 167–171.

The problem of determining the equilibrium composition of the gas phase from the known composition of the liquid phase is analyzed in terms of the Redlich–Kwong–Soave equation of state modified by Wang. An effective algorithm is suggested for solving this problem for systems with an arbitrary number of components. The molecular-weight distribution of the Fischer–Tropsch synthesis products can be estimated by calculating the composition of the gas phase from composition data for the liquid phase resulting from the reaction.

MOTION OF PARTICLES THROUGH THE FIXED BED IN A GAS–SOLID–SOLID DOWNFLOW REACTOR

L.V. Barysheva, E.S. Borisova, V.M. Khanaev, V.A. Kuzmin, I.A. Zolotarskii, N.A. Pakhomov, A.S. Noskov

Chem. Eng. J., 91(2-3) (2003) pp. 219–225.

The experimental studies and mathematical modeling are presented for the residence time distribution of fine solids moving in a co-current downflow fixed-bed reactor. Experiments were carried at ambient conditions using a glass column of 30 mm i.d. packed by spheres of 4–6 mm diameter. Fine alumina of 50–250 μm was used as a moving solids. Solids flow rate was varied from 0.1 to 0.5 g cm^{-2} s^{-1}. The new flight-time technique is applied to measure residence time of fine particles in a packed bed. The influence of particle size and flow rate on the particles residence time is experimentally investigated. New three-dimensional model of moving of fine particles in a packed bed is developed. The model is based on the statistical calculations of an individual particle path in a packed column. Model validation was checked by comparing experimental values of particles residence time distribution with calculated one. Calculated values of particles residence time were found to be in a good agreement with experimental data at the solids flow rate below 0.1 g cm^{-2} s^{-1}.

RADIAL HEAT TRANSFER IN PACKED BEDS OF SPHERES, CYLINDERS AND RASHIG RINGS VERIFICATION OF MODEL WITH A LINEAR VARIATION OF λ_{er} IN THE VICINITY OF THE WALL

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Chem. Eng. J., 91(2-3) (2003) pp. 243–248.

Experimental data on the effective radial thermal conductivities and wall heat transfer coefficients of cylindrical beds formed of spheres, cylinders and Rashig rings are presented. The obtained heat transport parameters are compared with literature data. A model with a linear variation of λ_{er} in the vicinity of the wall is proposed to the description of the radial heat transfer in the packed bed. The model allows simple correlation between the wall Nusselt number and the bed core effective radial thermal conductivity. The model is verified by experiments.

CFD SIMULATION OF "GAUZE PAD–HONEYCOMB" CATALYTIC SYSTEM

V.P. Zakharov, I.A. Zolotarskii, V.A. Kuzmin

Chem. Eng. J., 91(2-3) (2003) pp. 249–255.

The paper is devoted to studies of gas flows and mass transfer in a two-stage catalytic system recently applied in ammonia oxidation at nitric acid plants. Numerical studies are performed by reducing a system to a flat-periodical set of slit channels. Mathematical model based on two-dimensional Navier–Stokes equations with periodicity boundary conditions is used. Dependence of a system performance on a distance between stages is investigated and found to have a non-monotonous character.

RATE-DETERMINING STEPS, RATE-DETERMINING PARAMETERS, AND APPARENT ACTIVATION ENERGY OF STEPWISE REACTIONS.
1. STEPWISE NON-CATALYTIC REACTIONS LINEAR IN RESPECT TO INTERMEDIATES

V.N. Parmon

React. Kinet. Catal. Lett.,
78(1) (2003) pp. 139–150.

The paper considers a mathematically correct approach to define the rate-determining steps, rate-determining parameters as well as the apparent activation energy for steady occurrence of stepwise reactions with a known reaction scheme. Examples of the application of the suggested approach to analysis of simple stepwise reactions linear in respect to intermediates are presented.

RATE-LIMITING STEPS, RATE-DETERMINING PARAMETERS, AND APPARENT ACTIVATION ENERGY OF STEPWISE REACTIONS.
2. SIMPLE STEPWISE CONSECUTIVE CATALYTIC REACTIONS LINEAR IN RESPECT TO INTERMEDIATES

V.N. Parmon

React. Kinet. Catal. Lett.,
79(2) (2003) pp. 303–317.

The paper considers the application of a recently suggested mathematically correct approach for determining the rate-limiting steps, rate-determining parameters as well as the apparent activation energy for the steady occurrence of simple stepwise consecutive catalytic reactions which are linear in respect to catalytic intermediates. Under consideration are situations of both the small and large coverage of the surface with catalytic intermediates.

MATHEMATICAL MODELING OF CATALYTIC PROCESSES OVER UNSTEADY-STATE CATALYSTS: TWO-REACTOR SYSTEM

S.I. Reshetnikov, E.A. Ivanov

Siberian J. Industrial Math.,
6(13) (2003) pp. 108–117.

Mathematical modeling of heterogeneous reactions in a two-reactor system with circulating catalysts is fulfilled. It is based on a kinetic model and takes into consideration two types of catalytic centers. An effect of various parameters, such as reagent concentrations, catalyst volumes ratio, rate of catalyst circulation are studied. It is shown, that performance of the catalytic process over unsteady-state catalyst results in essential increase of desired product yield in comparison with a one-reactor system.

NONEQUILIBRIUM THERMODYNAMICS OF AUTOWAVES OF LAMINAR COMBUSTION IN A REVERSIBLY REACTING MEDIUM

A.P. Gerasev

Combust., Explos., Shock Waves,
39(4) (2003) pp. 423–430.

Thermodynamics of physicochemical processes in a reversibly reacting distributed kinetic system is considered, and nonequilibrium entropy of autowaves of laminar combustion is constructed. A qualitative and numerical analysis of the local and total entropy production in the system is performed. The total entropy production is shown to be a functional on integral curves, possessing extreme properties, whose minimum corresponds to the only physically meaningful solution of the problem. The results of solving problems with kinetic equations that take into account the reversible or irreversible character of the chemical reaction are compared.

NUMERICAL SIMULATION OF N-BODY GRAVITATIONAL DYNAMICS BY PIC METHOD: A PARALLEL IMPLEMENTATION

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Siberian J. Numer. Math., 6(1) (2003) pp. 25–39.

The evolution of self-gravitating systems such as the accretion discs is of great interest to astrophysics. The aim of this work is to create a parallel program for the accretion disc simulation on high-performance multiprocessor computers. The disc structure formation is N-body problem in a self-consistent gravity field. A good approximation to the problem is the Vlasov-Liouville kinetic equation. In the present work, the equation is solved by the PIC method. The main difficulty here is the evaluation of gravitational potential, which is given by the 3D Poisson equation. The parallel scheme of the algorithm was designed for the MIMD computers in an assembly technology. This means that the program is assembled of minimal fragments, each being a ready-made program containing potential values and the particles from one or more grid layers. The values of a grid potential are uniformly distributed among the processor elements uniformly in the radial direction. As the potential evaluation takes the main time, the distribution of particles is of minor importance here. Test computations conducted on the ICT cluster of Pentium-III workstations showed the linear acceleration as compared to the sequential version.

STUDY OF THE INSTABILITIES OF COLLISIONLESS SYSTEMS ON THE BASIS OF STOCHASTIC TRAJECTORIES

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(*Institute of Computer Technologies, Novosibirsk, Russia; **Budker Institute of Nuclear Physics, Novosibirsk, Russia)

JETP Lett., 78(6) (2003) pp. 358–362.

A practical method for distinguishing stochastic and regular subsystems in the entire set of particles for numerical modeling of the development of physical instabilities in collisionless systems with self-consistent fields is proposed. The method of subdividing the phase space into subsystems is based on the comparison of the results of two computational experiments with identical initial conditions but different realizations of rounding errors. An example of establishing the spatial and temporal domains of the development of collective instability and determining the instability increments is offered by a gravitating disk.

A NEW CONCEPT REACTOR FOR HYDROCARBON HYDROGENATION IN THE REACTIVE EVAPORATION MODE

N.A. Kuzin, A.V. Kulikov, A.B. Shigarov, V.A. Kirillov

Catal. Today, 79-80(1) (2003) pp. 105–111.

A new gas–liquid–solid reactor is presented whose concept is based on the coupling of liquid imbibition, evaporation, and an exothermic gas-phase reaction within a non-permselective catalytic porous membrane. Because of enhanced thermal conductivity of the sintered metal catalyst support and liquid flow re-circulation, it is possible to eliminate hot spots and runaways and to maintain high productivity of the reactor. When vapor conversion in the membrane is high, the problem of separation of the product from the gas phase reduces to common condensation. The preliminary experiments on the α-methylstyrene (AMS) hydrogenation on the 10 % (0.9 % Pd/γ-Al_2O_3) + 90 % (80 % Ni, 20 % Al) membrane sintered on the tube wall are very promising, however, further investigations are required.

THERMALLY COUPLED CATALYTIC REACTOR FOR STEAM REFORMING OF METHANE AND LIQUID HYDROCARBONS: EXPERIMENT AND MATHEMATICAL MODELING

V.A. Kirillov, N.A. Kuzin, A.V. Kulikov,
S.I. Fadeev*, A.B. Shigarov, V.A. Sobyanin
(*Sobolev Institute of Mathematics, Novosibirsk, Russia)

Theor. Found. Chem. Eng., 37(3) (2003) pp. 276–285.

An energy-efficient catalytic reactor for producing synthesis gas from methane and liquid hydrocarbons is proposed that is based on the coupling of an endothermic reaction (steam reforming of methane, hexane, or isooctane) and an exothermic reaction (hydrogen oxidation by atmospheric oxygen) in a single cocurrent apparatus. To describe the processes in such an apparatus, a two-dimensional two-temperature mathematical model is developed. It was revealed experimentally and by mathematical modeling that the heat- and mass-transfer coefficients of the gas flow in contact with the catalytically active wall in the exothermic reaction zone considerably affect the thermal conditions in the reactor.

ELEVATION OF PERFORMANCE OF GAS–LIQUID REACTORS ON SOLID CATALYST

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V.A. Semikolenov, I.V. Kuchin*, O.P. Zhukova*
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Chem. Eng. J., 91(2-3) (2003) pp. 199–204.

Different kinds of initial conditions for the gas–liquid process on a solid catalyst are discussed in the paper. The advantages of process with preliminary saturation of liquid with gas are considered. For the liquid batch reactor it is theoretically shown that preliminary saturation of the initial solution with gas prior to reaction profits more in comparison with "usual" mode. The experiments on hydrogenation of ethyl ether of *p*-nitrobenzoic acid to anesthesyne on suspended 5 % Pd/C catalyst in a batch reactor were carried out for verification of the main results from the proposed model ($P_{H2} = 40$ bar, $T = 20–120$ °C). As an example of a reactor, where the preliminary saturation effect can be used, the trickle-bed reactor operating without pumping was considered. Mathematical simulation of such type reactor is presented.

DEVELOPMENT AND TESTING OF SPECIAL METHODS OF CATALYST LOADING. APPLICATION IN HYDROTREATING AND REFORMING REACTORS

O.P. Klenov, A.S. Noskov

Catal. Ind., 2 (2003) pp. 67–73.

It was shown that the conditions of formation of a stationary layer in the course of catalyst loading into the reactor affect the main characteristics of the layer: apparent density, hydraulic resistance, and distribution of the flow being filtered within the layer volume. Finally, this determines the effectiveness and duration of catalyst operation. The processes and installations were developed for charging of granulated catalyst in multiple-shell and radial reactors providing the formation of apparent layers with uniform bulk structure. Their experimental validation has been made on the stands. Charging was executed into the industrial reforming and hydraulic refining reactors at a series of refineries as well as into the installations for ammonia and methanol production. Some results related to loading processes into the industrial reactors are shown: increase in apparent density and quantity of loaded catalyst by 8–12 %, noticeable decrease in the layer shrinkage in the course of operation, more uniform catalyst deactivation across the reactor section. A comparison is carried out with known processes of dense charge.

STUDIES ON THE ONSET VELOCITY OF TURBULENT FLUIDIZATION FOR ALPHA-ALUMINA PARTICLES

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Chem. Eng. J., 91(2-3) (2003) pp. 215–218.

Transition from bubbling to turbulent fluidization regime for alpha-alumina particles was experimentally studied in the 0.15 m i.d. cold flow model. Experiments were carried out at 1 atm and ambient temperature. Both standard deviation and amplitude spectra analysis were used to determine the transition. Transition velocity of 0.8 m/s was obtained for the particles under investigation.

THE EFFECT OF THE CATALYTIC LAYER DESIGN ON OXIDATIVE DEHYDROGENATION OF PROPANE OVER MONOLITHS AT SHORT CONTACT TIMES

S.N. Pavlova, V.A. Sadykov, Yu.V. Frolova, N.F. Saputina, P.M. Vedenikin, I.A. Zolotarskii, V.A. Kuzmin

Chem. Eng. J., 91(2-3) (2003) pp. 227–234.

Main factors determining performance of straight channel corundum monolith supported catalysts in the autothermal reaction of propane oxidative dehydrogenation at short contact times are verified. It was made possible by using a unique design of the catalytic reactor which allows an independent tuning of the gas preheat temperature and the catalyst temperature. It is also equipped with a cooled sampler to cut any homogeneous reactions after the catalyst layer. The effects of the front and back thermal shields, feed rate, relative contact time and the void space between the catalytic monoliths or after them are elucidated. The performance of the monolithic catalyst is compared with that crushed and packed into a granulated layer. A substantial impact of the homogeneous gas-phase reactions on the propane conversion and product selectivities is demonstrated. In turn, their share depends upon the longitudinal temperature gradient within the monolithic layer as determined by the heat generation in the inlet part due to propane combustion by oxygen, its transfer along the monolith layer and consumption in the rear part of the monolith in the absence of oxygen through endothermic reactions of dehydrogenation, cracking and steam reforming. In the autothermal mode of the propane oxidative dehydrogenation at short contact times on monolithic catalysts, the effect of those factors is as important as that of the catalyst and feed chemical composition.

AMMONIA OXIDATION INTO NITROUS OXIDE OVER Mn/Bi/Al CATALYST.
1. SINGLE COOLING TUBE EXPERIMENTS

A.S. Noskov, I.A. Zolotarskii, S.A. Pokrovskaya, V.N. Korotkikh, E.M. Slavinskaya, V.V. Mokrinskii, V.N. Kashkin

Chem. Eng. J., 91(2-3) (2003) pp. 235–242.

The process of ammonia oxidation with air oxygen was tested on the pilot-scale using a single-tube reactor to model the unit of a multi-tubular industrial reactor. The spherical Mn/Bi/Al catalyst was loaded into the reactor tube. Experimental studies were based on the data obtained by kinetic studies and simulation of the tubular reactor. The relationship between the operation conditions and temperature regime was established by varying the process parameters over a wide range. The steady-state temperature regimes were observed at the inlet ammonia concentration equal to 4–5 %. The selectivities to nitrous oxide and nitrogen oxide reached 87–88 % and no more than 0.5 %, respectively, at near 100 % conversion of ammonia.

Modeling of the pilot reactor demonstrated a good agreement between the experimental and calculated data that supports appropriateness of the reactor simulation for prediction of technological regimes for the industrial reactor. The Rashig rings loaded in the tubular reactor were found to provide stable operation regimes at the inlet ammonia concentration of 7–8 %.

STUDY OF CATALYSTS FOR CATALYTIC BURNERS FOR FUEL CELL POWER PLANT REFORMERS

Z.R. Ismagilov, M.A. Kerzhentsev, V.A. Sazonov, L.T. Tsykoza, N.V. Shikina, V.V. Kuznetsov, V.A. Ushakov, S.V. Mishanin*, N.G. Kozhukhar*, G. Russo, O. Deutschmann**** (*Russian Federal Nuclear Center - All-Russian Research Institute of Experimental Physics, Sarov, Russia; **Instituto di Ricerhe sulla Combustione, Napoli, Italia; ***University of Heidelberg, Heidelburg, Germany)

Korean J. Chem. Eng., 20(3) (2003) pp. 461–467.

Catalytic burners for fuel cell power plant reformers are alternative to conventional flame burners. Their application is expected to provide uniform temperatures in the reformer, efficient use of low-calorific gaseous by-products and reduction of pollutant emissions. For testing in the burners, a series of spherical $Pd/CeO_2/Al_2O_3$ catalysts were prepared. An optimum concentration of ceria providing the highest thermal stability of catalysts was determined. An effect of catalyst activation in the reaction mixture – 1 % methane in air was observed. A series of Mn containing oxide catalysts on spherical γ-Al_2O_3 or $(\gamma+\chi)$-Al_2O_3, both pure and doped with La, Ce and Mg oxides were prepared. The catalysts were characterized by chemical analysis, X-Ray phase analysis, BET surface area and activity measurements in methane oxidation. A batch of Mn-Mg-La-Al-O catalyst was prepared for further long-term testing in a model reformer with a catalytic burner. A model reformer with a catalytic burner was designed and fabricated for testing in the composition of the bench-scale Fuel Cell Power

Plant. Preliminary testing of this catalyst showed that it provided complete methane combustion at the specified operational temperatures over 900 °C.

COMBUSTION AND PROCESSING OF RICE HUSK IN THE VIBROFLUIDIZED BED OF CATALYST OR INERT MATERIAL

A.D. Simonov, T.I. Mischenko, N.A. Yazykov, V.N. Parmon

Chem. Sustain. Devel., 11(1) (2003) pp. 277–284.

In the present work, some data on catalytic combustion of one of the most widespread vegetative remainders – rice husk are adduced. The rice husk is used not only as a fuel, but also as a source of silicon for semiconductor industry, the synthesis of silicon carbides and silicon nitrides, *etc*. The rice husk oxidation in the vibrofluidized bed of either a catalyst or an inert material has been studied in conditions allowing to reproduce with an adequate accuracy the data on scraps combustion in the dense and unloaded phase of the fluidized bed. It is found that the process of the rice husk combustion is localized completely in the bed of the catalyst. In the bed of an inert material the process occurs in a space above the bed; consequently, exhausts contain a fair quantity of CO. Studies on solid products of the rice husk combustion have shown that their texture is determined mainly by silica, which is contained in rice husk as amorphous silica $SiO_2 \times nH_2O$. The adsorption ability of these solid products in respect to methylene blue (MB) is investigated. With increasing the process temperature, the value of limiting MB adsorption by the solid products passes through a maximum at the process temperature 600 °C. It is found that the values of the limiting MB adsorption for the solid combustion products in the bed of the catalyst exceed those for solid products obtained in the bed of an inert material. Under discussion are also some distinctions of the process of rice husk processing in the vibrofluidized beds of either catalyst or inert material.

FUEL COMBUSTION IN THE FLUIDIZED BED OF AN INERT MATERIAL WITH AN UNMOVABLE CATALYTIC SMALL-VOLUME PACKAGE

N.A. Yazykov, A.D. Simonov, T.I. Mischenko, A.S. Aflyatunov, S.V. Smolin, V.N. Parmon

Chem. Sustain. Devel., 11(1) (2003) pp. 321–326.

The capability of combustion of solid fuels (such as the brown coal of the Kansk-Achinsk coal deposit) in the fluidized bed of an inert material in the presence of unmovable catalytic packages is investigated. This arrangement of the catalytic process is shown to allow the achievement of the same parameters of the fuel burn off and the content of toxic substances in the flue gas as in the case of fuel combustion in the fluidized bed of catalyst grains. The new arrangement of catalytic processes can be recommended for the accomplishing of some other exothermic catalytic reactions, which require the maintenance of isothermal conditions.

MICROSPHERES OF FLY ASH AS A SOURCE FOR CATALYTIC SUPPORTS, ADSORBENTS AND CATALYSTS

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Chem. Sustain. Devel., 11(1) (2003) pp. 303–308.

The present paper reviews the processes of separation of microspheres from fly ash and their possible applications for the creation of catalytic supports, adsorbents and catalysts. To isolate magnetic microspheres and cenospheres of stabilized composition, the process flowsheets of concentrate separation, based on the combination of hydro- or aerodynamic and granulometric classification, followed by the separation in magnetic field of different intensity, were developed. Novel materials based on cenospheres of stabilized composition, such as mesoporous microspherical glasses (specific surface area S_{sp} = 3–50 m^2/g), the supported iron oxide systems (S_{sp} = 50–200 m^2/g), and zeolites are described. Spherical zeolites demonstrated good ion exchange properties in cesium and strontium removal from the technological solutions. The catalytic properties of Fe_2O_3/cenosphere catalysts and magnetic microspheres in deep oxidation of methane are discussed.

CATALYTIC HEAT GENERATING ELEMENT FOR AUTONOMOUS DOMESTIC HEATING SYSTEMS

B.N. Lukyanov, V.A. Kirillov, N.A. Kuzin, M.M. Danilova, A.V. Kulikov, A.B. Shigarov

Chem. Eng. J., 91(2-3) (2003) pp. 191–198.

New heat-conducting metal porous reinforced catalysts were developed to manufacture a catalytic heat generating element (CHGE) of 25 kW power. The element was subjected to thermophysical, hydraulic and ecological testing. Local temperature and gas flow rates were determined in different places of the outer catalytic bed surface. The impact of the convective and radiant transfer in total CHGE heat generation have been estimated.

Dynamics of CHGE startup was studied. A prototype of the catalytic water boiler supplied with a CHGE of 25 kW power was manufactured and tested. The boiler provides below yield of toxic waste: CO 5–10 ppm, NO_x traces, CH_4 10–20 ppm, CO_2 10 vol. %, the other gases 89.5 vol. %. CHGE is promising as a device for ecologically safe heat production for household appliances.

A 25-kW HOT-WATER HOUSEHOLD BOILER OPERATING ON THE PRINCIPLE OF CATALYTIC OXIDATION OF NATURAL GAS

N.A. Kuzin, V.A. Kirillov, V.A. Kulikov, B.N. Lukyanov, I.A. Onufriev, A.B. Shigarov

Therm. Eng., 49(8) (2002) pp. 648–655.

The basic possibility of creating new efficient and environmentally friendly water-heating devices operating in accordance with the principle of direct complete catalytic oxidation of natural gas is shown. New heat conducting porous-metal catalysts have been developed for its realization; the construction of a 25 kW heating element has been created and tested, and on its basis, a pilot hot-water boiler using natural gas as the fuel has been made.

FLAMELESS CATALYTIC COMBUSTION IS A PROMISING METHOD TO BOOST THE EFFICIENCY OF FUEL COMBUSTION AND TO MINIMIZE HARMFUL WASTES

V.N. Parmon, Z.R. Ismagilov, V.A. Kirillov, A.D. Simonov

Energy Saving and Energetics in Omsk Region, 2(7) (2003) pp. 74–78.

BIC's technology of two-stage catalytic combustion of hydrocarbon fuels is used to generate sanitary clean hot air. The principle underlies functioning of catalytic hot air generators. For utilization of the calorific value of energy carriers, the efficiency factor is no less than 99 %.

Catalytic heaters ("electric fireplaces" or "convectors") for heating living quarters and industrial buildings are designed at BIC and industrially implemented in Russia. They are fueled by hydrocarbon gases. The advantages are fire and ecological safety, small dimensions and mobility, more economic heat production in comparison to electric heating.

SEPARATION OF THE TRIBUTYL PHOSPHATE – KEROSENE EXTRACTION MIXTURE USING FORMIC ACID

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Radiochem., 45(4) (2003) pp. 367–370.

Separation of the TBP-kerosene extraction mixture using formic acid was studied, and the optimal process parameters were determined. The experimental data strongly suggest formation of the solvate $(C_4H_9O)_3PO\cdot 3HCOOH$. The thorium distribution in separation of the TBP-kerosene mixture into two phases was studied.

Study of Nucleation Processes

NUCLEATION: THEORY AND EXPERIMENT

M.P. Anisimov

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Various theoretical and experimental methods used to study nucleation are considered. Since theoretical methods have some fundamental limitations, lacking information is usually gained from experimental research. It is demonstrated that the nucleation theory is at the beginning of the new stage of development which is going to be, in essence, semiempirical. A semiempirical method for constructing nucleation rate surfaces is described. The topology of these surfaces in the limit of zero nucleation rate can be determined using phase equilibration diagrams. This opens up the way for revising some approximations applied in experiments and some axioms of the classical nucleation theory. Some examples of practical use of nucleation essential for the development of modern technology are given (Bibliography – 396 references).

CORRELATIONS FOR VAPOR NUCLEATING CRITICAL EMBRYO PARAMETERS

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J. Phys. Chem. Ref. Data,
32(4) (2003) pp. 1387–1410.

Condensation Nucleation Light Scattering Detection in principle works by converting the effluent of the chromatographic separation into an aerosol and then selectively evaporating the mobile phase, leaving less volatile analytes and nonvolatile impurities as dry aerosol particles. The dry particles produced are then exposed to an environment that is saturated with the vapors of an organic solvent (commonly n-butanol). The blend of aerosol particles and organic vapor is then cooled so that conditions of vapor supersaturation are achieved. In principle, the vapor then condenses onto the dry particles, growing each particle (ideally) from as small as a few nanometers in diameter into a droplet with a diameter up to about 10 µm. The grown droplets are then passed through a beam of light, and the light scattered by the droplets is detected and used as the detector response. This growth and detection step is generally carried out using commercial continuous-flow condensation nucleus counters. In the present research, the possibility of using other fluids than the commonly used n-butanol is investigated. The Kelvin equation and the Nucleation Theorem (Anisimov *et al.*, 1978) are used to evaluate a range of fluids for efficacy of growing small particles by condensation nucleation. Using the available experimental data on vapor nucleation, the correlations of Kelvin diameters (the critical embryo sizes) and the bulk surface tension with dielectric constants of working liquids are found. A simple method for choosing the most efficient fluid, within a class of fluids, for growth of small particles is suggested (Bibliograpy – 76 references).

GENERAL REQUIREMENTS AND RECOMMENDATIONS FOR VAPOR NUCLEATION RATE EXPERIMENTS

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Aerosol Sci. Technol., 37(2) (2003) pp. 183–186.

Agreement between experimentally measured vapor nucleation rates and current theoretical predictions exists for only a limited number of systems. These inconsistencies can result from differences in measurement methods and assumptions used to interpret the experimental results. Usually the causes of these disagreements are unclear. The current state of the art is such that experimental results using different methods can lead to very different interpretations of the same phenomenon. In this note, well-defined standard systems are suggested as a means to verify experimental system performance. The combination n-pentanol-helium is suggested as a standard reference system. Using this system, measurements produced by multiple research groups have been compiled, and from these experimental results, a nucleation rate equation was developed that can serve as a standard basis for method comparison. This equation provides a scale to relate nucleation rates over a range of nucleation temperatures and is a useful basis of comparison even if the proposed equation is not fully accurate. It is further suggested that the nucleation rate measurements be performed using small steps in nucleation temperature of around 2° or less to identify the features in the system such as phase changes in the critical embryos. In this note, a method that uses monotonicity and continuity conditions for the nucleation rate surface to detect such singularities is outlined. These monotonicity and continuity criteria can be formulated as a dimensionless quantity. The semiempirical construction of nucleation rate surfaces can indicate conditions where multiple nucleation rate surfaces may be detected. Experimental systems that include size distribution measurements have the potential to discern particles produced through multiple nucleation channels such that nucleation rates can be measured for each channel. Detection of nucleation rate surface singularities is important because these singularities indicate the existence of two-channel nucleation where one-channel nucleation theory cannot be applied.

Catalysis for Petrochemical Industry

DOMESTIC OIL-REFINING INDUSTRY IN THE LIGHT OF CATALYSIS. THE STATE AND PROBLEMS

V.N. Parmon, V.K. Duplyakin

Catal. Ind., 2 (2003) pp. 3–10.

The paper gives a review of the state in the oil-refining industry of Russia in the view of general tendencies in the world now and in prospect in relation of oil production and oil refining level. The main strategic objectives are considered which are related to the rational use of oil stock, relation of scales and priority of execution of the objectives determining the further modernization of the refineries and, first of all, engineering solutions in the field of catalysis and the processes of single catalytic stages, taking up-to-date demands to the level of oil processing, product range, and quality of target production into account.

CATALYTIC REFORMING. PRESENT-DAY STATE IN DOMESTIC AND FOREIGN OIL-REFINING INDUSTRY

A.S. Bely

Catal. Ind., 2 (2003) pp. 11–19.

An analysis of up-to-date state concerning the process of catalytic gasoline-fraction reforming is given. Comparative data of the executing conditions and effectiveness of different versions of known processes as well as their distribution in Russia and abroad are discussed. The results of experience gained during reconstruction and modernization of industrial reforming plants with periodic catalyst regeneration are generalized. The state of the catalyst production in the country and the economic situation in the catalyst market is presented. Based on available experience of industrial operation, the results of comparative estimations of effectiveness of import and new Russian catalysts are cited.

IMPROVEMENT OF REFORMING CATALYSTS AND PRODUCTION PROCESS. NEW DEVELOPMENTS OF THE CATALYSIS INSTITUTE

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Catal. Ind., 6 (2003) pp. 3–12.

The paper summarizes the results of fundamental investigations concerned the nature of active surface of reforming catalysts and expounds the concepts of the further progress in the field of designing of catalysts and the reforming process. The developed conceptual views of the design of active surface have been realized in industrial PR series catalysts. The given summary of the industrial operation of developed catalysts demonstrates effectiveness of the proposed approach for improvement of industrial catalyst compositions in order to increase selectivity of paraffin hydrocarbon aromatization. The technical properties of new catalyst grades and the variants of modernization of standard reforming plants for increasing the effectiveness of their operation are discussed.

DOMESTIC MICROSPHEROIDAL CATALYSTS FOR CRACKING. EXPERIENCE OF DEVELOPMENT AND APPLICATION

V.P. Doronin, T.P. Sorokina, V.K. Duplyakin, V.N. Parmon, V.I. Gordenko, V.V. Khrapov

Catal. Ind., 2 (2003) pp. 37–48.

The main approaches to development of industrial catalysts for oil stock cracking are described. The requirements to the components of cracking catalysts are formulated and developed methods for realization of the requirements are demonstrated. The scientific fundamentals of synthesis process and modification of the zeolite component of a catalyst and the principles to create wide-porous composite matrices for zeolite-bearing catalysts are considered. The fundamentals of the catalyst production and operation in industrial plants of catalytic cracking of 43–103 and 43–107 type of deep processing of KT-1/1 oil residue are considered.

INFLUENCE OF CAPSULATION IN THE MATRIX Al_2O_3/Al OF INTERMETALLIDES $ZrFe_2$, TREATED IN HYDROGEN

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Petroleum Chem., 43(6) (2003) pp. 379–382.

A Fischer–Tropsch catalyst is proposed, the $ZrFe_2$ intermetallide treated with hydrogen and encapsulated in the Al_2O_3/Al matrix formed under hydrothermal conditions. This composite catalyst is characterized by a considerable increase in the specific turnover capacity of $ZrFe_2$, probably due to both structural (small size of encapsulated particles, particular pattern of the porous structure) and chemical factors (changes in the $ZrFe_2$ surface due to oxidation during hydrothermal treatment, interaction with the matrix material).

FISCHER–TROPSCH SYNTHESIS USING A POROUS CATALYST PACKING: EXPERIMENTAL EVIDENCE OF AN EFFICIENT USE OF PERMEABLE COMPOSITE MONOLITHS AS A NOVEL TYPE OF THE FISCHER–TROPSCH SYNTHESIS CATALYST

A.A. Khassin, T.M. Yurieva, A.G. Sipatrov, V.A. Kirillov, G.K. Chermashentseva, V.N. Parmon

Catal. Today, 79-80(1) (2003) pp. 465–470.

Novel type of the catalytic material: a permeable composite monolith (PCM) is studied in the Fischer–Tropsch synthesis (FTS) at 2.1 MPa. Due to highly intense mass transfer and high density of an active component, it was shown to provide steadily the process productivity of ca. 100–200 mg/(hcm^3) of reactor volume at 483 K. At that the selectivity of the process over PCM is maintained at the highest level ($\alpha = 0.84$; the olefin fraction in the C_3–C_4 fraction above 50 %). At the effective mode of the PCM particle operation, the effectiveness factor of ca. 70 % is achieved.

FISCHER-TROPSCH SYNTHESIS USING POROUS CATALYST PACKING. FEASIBILITY STUDY OF PERFORMING MULTIPHASE CATALYTIC PROCESS USING PERMEABLE COMPOSITE MONOLITHS

A.G. Sipatrov, A.A. Khassin, T.M. Yurieva, V.A. Kirillov, G.K. Chermashentseva, V.N. Parmon

Chem. Sust. Devel., 11(1) (2003) pp. 285–292.

A novel scheme for the organization of the three-phase process has been proposed, basing on a new type of a stochastically organized porous and catalytically active composite monolith (PCM). The high catalyst loading (1 g/cm^3) and high heat conductivity (3 W/(m K)) make this new material very attractive for exothermic multiphase processes, *e.g.* for the Fischer–Tropsch synthesis. The possibility of preparing strong PCMs with the permeability of 10–500 mDarcy has been demonstrated. The gas-vapor phase flow through a PCM particle can be performed via transport pores which diameter was measured as 4–10 mm. The pressure drop has been shown to be reasonable for the Fischer–Tropsch synthesis. The effectiveness of the PCM usage at 0.1MPa, 210 °C has been found to be above 70 %. PCM material was concluded to be the prospective.

BIMT: A NEW ENERGY-SAVING AND RESOURCE-SAVING TECHNOLOGY FOR PRODUCTION OF HIGH-QUALITY MOTOR FUELS FROM MIDDLE OIL DISTILLATES AND GAS CONDENSATES

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Catal. Ind., 2 (2003) pp. 60–66.

A nontraditional process has been developed in two versions: BIMT and BIMT-2 – one-stage catalytic refining of intermediate petroleum distillates or unstable gas condensates, including those with high contents of high-stable sulfur compounds of thiophenic series boiling off in the temperature range of 35-360 ºC, into high-octane gasoline, winter diesel fuel and condensed gas C_3-C_4. The process is carried out on zeolite catalysts IK-30-BIMT and IC-30–BIMT-2, which contain no noble metals, in reactors with stationary catalyst layer at $T = 350 \div 450$ ºC and $P <= 20$ at. The process permits simplifying significantly the now existing classic scheme of oil refining with simultaneous reducing some times the cost of production of the same products, i.e. high-quality motor fuels.

PRODUCTION OF 2,6-DIALKYLNAPHTHALENE - RAW MATERIAL FOR PRODUCTION OF POLYETHYLENE NAPHTHALATE

O.V. Komova, V.I. Simagina

Catal. Ind., 6 (2003) pp. 16–22.

Polyester material - polyethylene naphthalate (PEN), being new for the Russian market, is presented in this article. The properties and the application range of PEN are given. A review of the processes to produce 2,6-dialkylnaphthalens (2,6-DAN), which are basic raw materials for synthesis of the PEN, is considered. The main attention is paid to industrial production of 2,6-DAN. Significance of the catalytic routes of synthesis for development of industrial production of 2,6-DAN is shown.

APPLICATION OF POLYFUNCTIONAL CATALYSIS IN SYNTHESIS OF MOTOR FUELS FROM CO_2 AS AN APPROACH TO THE PROBLEM OF CO_2 UTILIZATION

V.M. Mysov, K.G. Ione

Chem. Sustain. Devel., 11(1) (2003) pp. 197–208.

The development of civilization is inevitably connected with the increase of energy consumption. Nowadays the main part of energy is produced through incineration of organic fuel, the products of fuel combustion (CO_2) being discharged into atmosphere. However the ecological problems impelled the world community to intensify their activity in order to decrease CO_2 emission. There is a great number of known chemical reactions, both catalytic and non-catalytic, which bound CO_2 chemically into various products. Specifically, the processes of hydrogen reduction of CO_2 may proceed with the production of methanol, dimethyl ether (DME), methane, light hydrocarbons, or liquid motor fuels. Among these, the processes of motor fuel production on the bi-functional catalysts are most likely to be industrially applied in a large scale. The scientific and technological aspects of the processes of hydrogen reduction of carbon dioxide are considered with regard to CO_2 utilization. The influences of the catalysts composition, pressure, temperature, $(H_2–CO_2)/(CO + CO_2)$ ratio, duration of the test run (up to 1000 h) on the activity and selectivity of the bi-functional catalysts in the synthesis of liquid motor fuels were studied. Depending on the composition of the liquid organic products, utilization of carbon in CO and CO_2 comprised 70 to 90 %.

PRODUCTION OF MOTOR FUELS AT THE PLANTS OF LOW AND MIDDLE CAPACITY USING "ZEOFORMING", A NEW CATALYTIC PROCESS

V.G. Stepanov, K.G. Ione

Catal. Ind., 2 (2003) pp. 49–59.

The paper examines the problems of producing motor fuels, namely motor gasoline and diesel fuels, from oil and gas condensate at small installations located near the oil and gas-condensate fields. In the most cases oil and gas condensates are shown to permit producing diesel fuel at the field installations by varying fractional compositions and using additives. Because of low octane numbers of the straight-run gasoline fractions, addition of antiknock agents to them in the quantities permitted by the standards does not enable one to produce motor gasoline, while the technique of high-octane additives requires large amounts of them. The catalytic processes permitting increasing the octane numbers of gasoline fractions are studied. A conclusion is made that the Zeoforming process using a new zeolite-containing catalysts IK-30 is economically and technologically most suitable for production of graded motor gasoline at the installations of low and medium capacity.

PROBLEMS OF COMMERCIAL PRODUCTION OF HYDROGEN AS COMPARED WITH THE PROBLEMS OF MINING OF NATURAL HYDROGEN AS MINERAL WEALTH

K.G. Ione

Chem. Sust. Devel., 11(6) (2003) pp. 901-917.

Hydrogen is produced for industrial needs via high-temperature transformations of natural hydrogen-containing raw materials – coal, natural gas, biomass – or via electrolysis of water. There are a number of publications which indicate that hydrogen as a free element on Earth is not consumed but the hydrogen outflow to the Earth surface goes on. There are discovered gas outflows in which the hydrogen content is 10 to 50 vol %. Supposedly, hydrogen may be as yet the main gas constituent at a certain depth but, due to its high reactivity, it enters reactions with oxygen and carbon to form water and the reactions of hydrogenation of carbon inclusions to form hydrocarbon fluids. Therefore, flow of hydrogen in the free state to the Earth surface cannot be intense. In the present review paper, the attempt is made to assess the strategic, technological and economic practicability of exploring, mining and concentrating natural hydrogen, as well as ecological advantages of natural hydrogen utilization in order to reduce carbon dioxide wastes.

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Vortex Centrifugal Bubbling Reactor (VCBR),
XVI All-Russian Conference on Chemical Reactors "CHEMREACTOR-16", June 17–20, Kazan, Russia. Abstracts, pp. 197–200.

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   March 8–15, Kirchberg, Austria. Conference Program, p. 47.

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All-Russian Scientific Youth Conference "Under the Badge of "Sigma", June 23–28, Omsk, Russia. Abstracts, p. 93.

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The Study of Electron States of Copper in Cu-ZSM-5 Catalysts,
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437. **S.A. Yashnik, V.V. Kuznetsov, Z.R. Ismagilov, (N.M. Danchenko, S.P. Denisov),**
Development of Monolithic Catalysts with Low Noble Metal Content for Diesel Vehicle Emission Control,
6th International Congress on Catalysis and Automotive Pollution Control, "CAPOC-VI", October 22-24, Brussels, Belgium. Abstracts, pp. 435–446.

438. **S.A. Yashnik, T.V. Larina, N.T. Vasenin, Z.R. Ismagilov, V.F. Anufrienko,**
The Study of Electron States of Copper in Cu-ZSM-5 Catalysts,
All-Russian Scientific Youth Conference "Under the Badge of "Sigma", June 23–28, Omsk, Russia. Abstracts.

439. **N.A. Yazykov, A.D. Simonov, T.I. Mishenko, A.S. Aflyatunov, S.V. Smolin, V.N. Parmon,**
Brown Coal Combustion in the Fluidized Bed of an Inert Material with an Unmovable Catalytic Small-Volume Package,
6th European Congress on Catalysis "EuropaCat-VI", August 31-September 4, Innsbruck, Austria. Abstracts, B3.144.

440. **I.V. Yudaev, D.F. Khabibulin,**
NMR Investigation of Zirconia Pillared Clays,
Ampere XI NMR School, June 1-6, Zakopane, Poland. Proceedings, p. 89.

441. **M.M. Yulikov, O.N. Martyanov, (K.A. Tarasov, V.P. Isupov), V.F. Yudanov,**
Superparamagnetic Resonance Investigation of Nanosized Metal Particles Dispersion Incapsulated into a Dielectric Matrix,
6th European Congress on Catalysis "EuropaCat-VI", August 31–September 4, Innsbruck, Austria. Abstracts, A2.160.

442. **S.M. Yunusov, E.S. Kalyuzhnya, B.L. Moroz, V.A. Likholobov, V.B. Shur,**
The Synergistic Acceleration of the Ammonia Synthesis over the $K_2[Fe_2(CO)_8]$+K/Sibunit Catalysts by Rhodium and Iridium,
Mark Vol'pin Memorial Symposium "Modern Trends in Organometallic and Catalytic Chemistry" May 18–23, Moscow, Russia. Abstracts, p. 135.

443. **A.N. Zagoruiko,**
Performance of Selective Catalytic Exothermic Reactions in the "Reversed Heat Wave" Mode: A Way to Improve Selectivity,
XVI International Conference on Chemical Reactors "Chemreactor-16", December 1–5, Berlin, Germany. Abstracts, pp. 202–204.

444. **A.N. Zagoruiko, (V.D. Glotov, N.N. Menyailov, Yu.N. Zhukov, V.M. Yankilevich), B.S. Bal'zhinimaev, (V.A. Chumachenko, T.A. Popova), L.G. Simonova,**
Pilot Tests of Platinum Fiberglass Catalysts at Real Gases of Sulphuric Acid Plant,
XVI All-Russian Conference on Chemical Reactors "CHEMREACTOR-16", June 17–20, Kazan, Russia. Abstracts, pp. 173–176.

445. **A.N. Zagoruiko, (V.D. Glotov, N.N. Meniailov, Yu.N. Zhukov, V.M. Yankilevich), B.S. Bal'zhinimaev, L.G. Simonova,**
Glass Fiber Catalysts for SO_2 Oxidation: Pilot Tests at Real Gases of Sulfuric Acid Plant,
XVI International Conference on Chemical Reactors "Chemreactor-16", December 1–5, Berlin, Germany. Abstracts, pp. 395–398.

446. **A.N. Zagoruiko, P.A. Kuznetsov, A.N. Startsev, M.V. Sidyakin,**
Adsorption-Catalytic Technologies for Desulfurization of Natural Gas in Fuel Processors,
2nd All-Russian Seminar "Fuel Cells and Fuel Cell Power Plants", June 29–July 2, Novosibirsk, Russia. Abstracts, pp. 159–161.

447. **A.N. Zagoruiko, (V.V. Mokrinskii),**
Non-Steady-State Approach to Steady-State Kinetics: Case Study of H_2S Oxidation by Oxygen,
XVI International Conference on Chemical Reactors "Chemreactor-16", December 1–5, Berlin, Germany. Abstracts, pp. 399–402.

448. **V.A. Zakharov,**
Recent Data on the Number of Active Centers and Propagation Rate Constants in Olefin Polymerization with Supported ZN Catalyst,
European Polymer Conference on Stereospecific Polymerization and Stereoregular Polymers, "EUPOC 2003", June 8–12, Milan, Italy.

449. **V.A. Zakharov,**
Ethylene Polymerization over Supported ZN Catalyst with Different Composition: Some Kinetic Peculiarities on the Base of Data on the Number of Active Centers and Propagation Rate Constants,
International Conference "Workshop on ZN Polymerization", October, Kanadzava, Japan.

450. **V.P. Zakharov, I.A. Zolotarskii,**
Numerical Investigation of a Catalytic Reaction in a Honeycomb Channel. Hydrodynamically Induced Local Concentration Oscillations,
4th Interrnational Conference on Unsteady-State Processes in Catalysis, "USPC-4", October 26–29, Montreal, Quebec, Canada. Abstracts, p. 30.

451. **S.G. Zavarukhin, G.G. Kuvshinov,**
Catalytic Synthesis of Nanofibrous Carbon from Methane in Isothermal Reactors of Different Types,
International Conference "Carbon'03", July 6–10, Oviedo, Spain. Abstracts, p. 175.

452. **G.M. Zhidomirov, N.A. Kachurovskaya, (R.A. van Santen),**
Model DFT Study of the Intermediates of Benzene to Phenol Oxidation by N_2O on High-Silica Zeolites,
Russian-American Seminar "Advances in the Understanding and Application of Catalysts", "AUAC-2003", May 28–30, Moscow, Russia. Abstracts, pp. 75–76.

453. **I.A. Zolotarskii, V.A. Sadykov, V.A. Kuzmin, Z.Yu. Vostrikov, L.N. Bobrova, L.L. Gogin, T.A. Nikoro, V.S. Lakhmostov, D.N. Sokolov, L.G. Pinaeva, S.N. Pavlova, O.I. Snegurenko, T.G. Kuznetsova, S.F. Tikhov, (O.F. Brizitskii, V.Ya. Terentiev, A.P. Khristolyubov),**
Technology of Autothermal Reforming of Hydrocarbon Fuels at Short Contact Times,
2nd All-Russian Seminar "Fuel Cells and Fuel Cell Power Plants", June 29–July 2, Novosibirsk, Russia.

454. **(V. Zyryanov, N. Uvarov), V.A. Sadykov, G.M. Alikina, (L. Ivashkevich, M. Ivanovskaya, S. Neophytides),**
Mechanochemical Synthesis, Structure and Properties of Nanocrystalline Metastable Perovskites and Fluorites for Solid Electrolyte Applications,
X Asia-Pacific Academy Materials (APAM) Topical Seminar and III Conference "Materials of Siberia" "Nanoscience and Technology", 2–6 June, Novosibirsk, Russia. Abstracts, p. 173.

455. **D.A. Zyuzin, E.M. Moroz, V.A. Sadykov, T.G. Kuznetsova, A.N. Shmakov,**
X-Ray Diffraction Study of Local Structure of Ceria-Samaria Mixed Oxides,
International Symposium "Order, Disorder and Properties of Oxides, "ODPO-2003",
September 8–11, Sochi, Russia. Abstracts, p. 126.

456. **D.A. Zyuzin, E.M. Moroz, V.A. Sadykov, T.G. Kuznetsova, Yu.V. Potapova**, **(S. Neophytides),**
X-Ray Diffraction Study of High-Dispersed Ceria-Samaria Mixed Oxides,
XIX Conference on Applied Crystallography, September 1–4, Krakow, Poland. Abstracts, p. 77.

AUTHOR'S INDEX

CONTENT

Annual Review
of Activities in Fundamental Areas

2003

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