BORESKOV INSTITUTE OF CATALYSIS

SIBERIAN BRANCH OF RUSSIAN ACADEMY OF SCIENCES

ANNUAL REVIEW 2000

ANNUAL REVIEW
of Activities in Fundamental Areas
2000

BOREKOV INSTITUTE OF CATALYSIS
SIBERIAN BRANCH OF RUSSIAN ACADEMY OF SCIENCES

Novosibirsk

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Dear Colleagues,

This is a real pleasure for me to present already the seventh issue of the Annual Review of the Boreskov Institute of Catalysis in the main fields of its academic and R&D activities covering the year 2000.

The Boreskov Institute of Catalysis is well known to experts in both academic and industrial catalysis not only in Russia and CIS, but also in many western and oriental countries. Since the sixties it has remained the largest chemical research institution in the Asian part of Russia having many deep and stable traditions and providing research in nearly all fields of catalysis. Its interests spread from the sophisticated purely academic research to the real applied problems, including commercial catalysts and catalytic technologies.

During the last decade according to numerous changes in Russia and its stepwise approach to the market economy, there were also some sufficient changes in the behavior and life of the Boreskov Institute of Catalysis. However, in spite of general instability in the country, the Institute could survive as a high quality specialized organization. Moreover, the intensity and quality of the research and engineering activity at the Institute became even higher. 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. Hope, the readers will feel that themselves, when comparing the materials of this and previous issues of the Annual Review.

The year 2000 was very important for the life of the Institute in many aspects. First of all, the Institute has condoned to sustain successfully in the extremely high financial instability of Russia in the mid of 1998. This appeared possible only due to a very high professional value of the Institute among the industries both in Russia and abroad that helped financial self-maintenance of the Institute. Thus, since 1996 nearly one quarter of the Institute's budget originates as royalties or license fees from the industries, mainly the western ones. The total income from the Russian and foreign industries into the overall budget of the Institute has approached the value of 75 % in 1999. Also, since the mid 1990’s there was established a really strategic partnership with some Russian and world leading industrial companies. The situation remained nearly the same for year 2000, an extremely important feature being a rapid growing of the collaboration with the Russian industries: the total income from the Russian industries has grown for that year by a factor of 3.

Since 1998 the Institute has been 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 Science and Technologies of the Russian Federation.

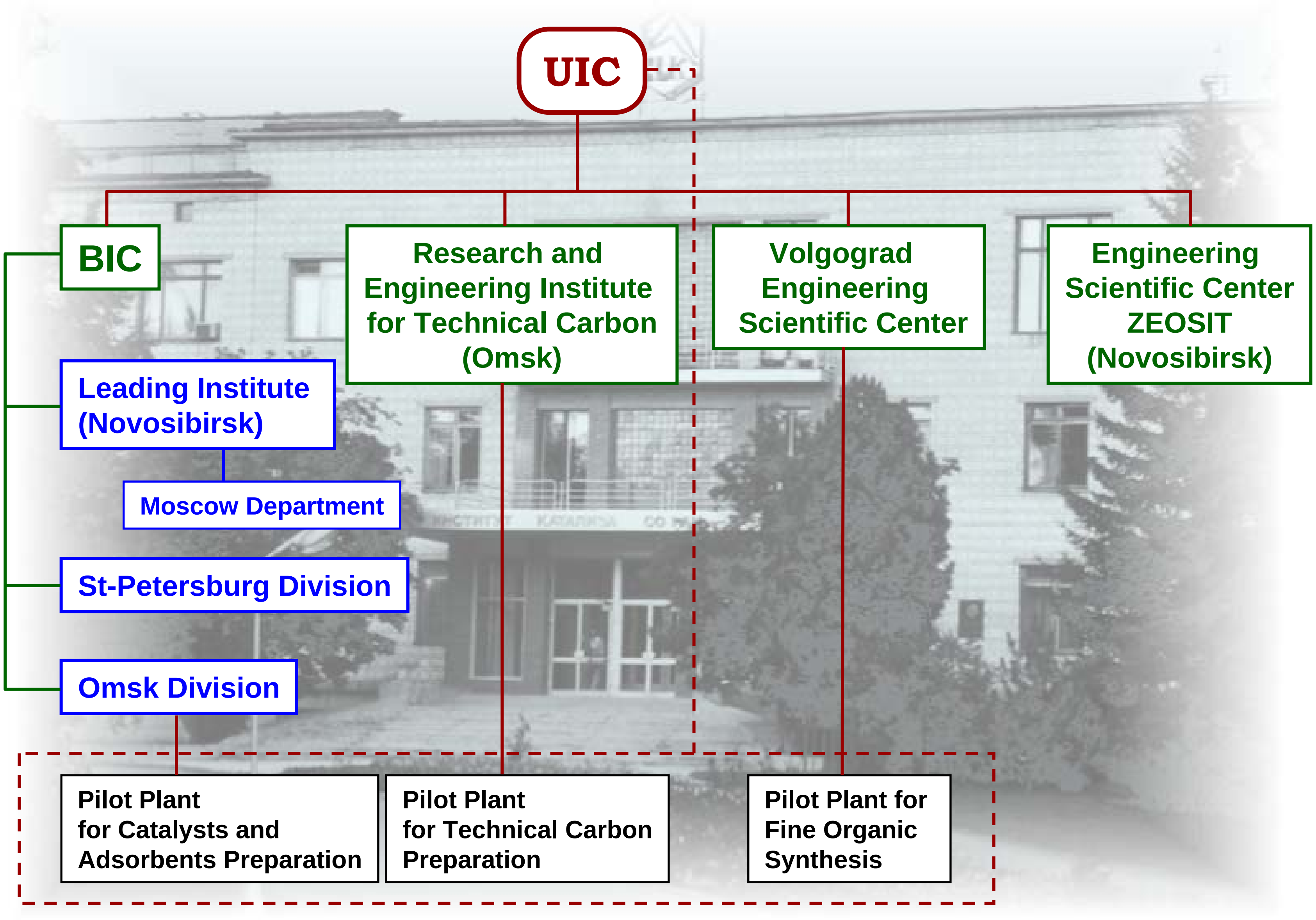
Since 1998 the Institute has been united with some other R&D chemical institutions of the Siberian Branch of the Russian Academy of Sciences in the frame of a new R&D association: the United Institute of Catalysis headed by the director of the Boreskov Institute of Catalysis. Now the United Institute 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. The facilities of the UOC include now three powerful pilot plants capable of providing manufacturing of the first industrial batches of various catalysts and specialty chemicals.

According to the Bylaw of both the Institute and the Russian Academy of Sciences, in the spring of 2000 there was accomplished a procedure of reelection of the Director of the Institute for the next five-year period. V. Parmon has remained the position of the Director. According to the Bylaw, the next step was the renovation also of the staff of both the Board of Directors as well as the Scientific Council of the Institute up to year 2005. Indeed, these changes were very important, since even now the main research and administrative management in the Institute belongs to a sufficiently young generation of researches. However, one can be sure that the management of the Institute is recognizing well all the existing problems taking the maintenance of high activity and productivity of R&D of the Institute in both fundamental and applied areas as the goals of the highest priority.

Hope this 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

United Institute of Catalysis (UIC)



UIC

BIC

Research and Engineering Institute for Technical Carbon (Omsk)

Volgograd Engineering Scientific Center

Engineering Scientific Center ZEOSIT (Novosibirsk)

Leading Institute (Novosibirsk)

Moscow Department

St-Petersburg Division

Omsk Division

Pilot Plant for Catalysts and Adsorbents Preparation

Pilot Plant for Technical Carbon Preparation

Pilot Plant for Fine Organic Synthesis

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, 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, of these 5 Corresponding Members of the RAS, more than 50 Professors, about 200 have a Ph.D. degree, and about 40 Ph.D. students. The Institute presents the unique society of 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 Problems, 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.

The Information Center was established to support WWW-server of the Institute http://www.catalysis.nsk.su and the United server SB RAS on Chemical Sciences http://www.catalysis.nsk.su/chem**.**

Data bank included 8 Databases on Russian and foreign catalysts, catalyst supports, catalytic processes, etc.

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

STRUCTURE OF THE INSTITUTE

Directorate:
S.E. Glaznev, S.P. Kil'dyashev, A.S. Noskov, V.A. Sobyanin, I.A. Kamolkin, O.N. Mart'yanov, V.A. Likholobov, R.A. Buyanov, V.N. Parmon, B.S. Bal'zhinimaev

DIRECTOR

Directorate

Scientific Council

Research Departments

DEPARTMENT OF PHYSICOCHEMICAL METHODS FOR CATALYST INVESTIGATION
8 laboratories and 5 groups Head: Prof. D.I. Kochubey

DEPARTMENT OF NONTRADITIONAL CATALYTIC PROCESSES AND TECHNOLOGIES
3 laboratories and 6 groups Head: Acad. V.N. Parmon

DEPARTMENT OF HETEROGENEOUS CATALYSIS
8 laboratories and 7 groups Head: Prof. V.A. Sobyanin

DEPARTMENT OF HOMOGENEOUS AND COORDINATION CATALYSIS
3 laboratories and 3 groups Head: Prof. V.A. Likholobov

DEPARTMENT OF EXPLORATORY AND APPLIED INVESTIGATIONS
2 laboratories and 4 groups, Center for Catalyst Characterization and Testing Head: Prof. Bair S. Bal'zhinimaev

DEPARTMENT OF CATALYTIC PROCESS ENGINEERING
8 laboratories and 1 group Head: Prof. A.S. Noskov

DEPARTMENT OF CATALYTIC PROCESSES OF FINE ORGANIC AND BIOORGANIC SYNTHESIS
2 groups Head: Aleksandr G. Tolstikov

DEPARTMENT OF APPLIED CATALYSIS PROBLEMS
Head: I.A. Zolotarskii

THE INFORMATION CENTER OF THE INSTITUTE
Head: Dr. V.L. Kuznetsov

Scientific-Supportive Units

Manufacturing Facilities

Administration and Services

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.

In the context of future research program, the Institute will continue to study the mechanisms and kinetics of actually important catalytic reactions, improve physicochemical and quantum-chemical methods used in catalysis, develop the research basis for purposeful synthesis of a number of catalysts, supports and sorbents (including non-traditional mechanochemical, plasma, radiation-thermal methods, etc.), study the regularities of formation of new materials (carbon-carbon composite materials of globular and fibrous structure, polymer-inorganic composites, composite membranes, etc.) as well as supports and adsorbents with the optimum geometry and controlled structure and mechanical properties (monolith multichannel ceramics, honeycomb carbon and ceramic monoliths); design new and improve the existing catalytic processes (cracking, alkylation, polymerization, etc.) and novel reactors, study the possibilities of using catalysis in such non-traditional fields as thermocatalytic conversion of solar and other types of energy; design of adsorption materials for freon-free air conditioners, accumulators of low-potential heat, active cooling systems; technologies with the use of low-energy fuels; various types of heaters with catalytic fuel cells, etc.

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 multicapillary columns
Superrapid chromatography
Mass-spectrometry

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

Porosimetry
Calorimetry

COMMERCIAL CATALYSTS AND TECHNOLOGIES OWNED BY THE BORESKOV INSTITUTE OF CATALYSIS

CATALYSTS FOR CONVERSION OF LIQUID ORTHO-HYDROGEN TO PARA-HYDROGEN

1970 - Uzbekistan

VANADIUM CATALYSTS FOR SULFURIC ACID PRODUCTION

1970 - Russia

CATALYSTS FOR ENVIRONMENTAL PROTECTION

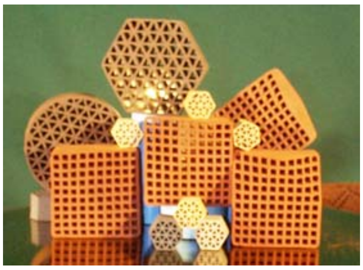
1990 - Russia

FORMALDEHYDE PRODUCTION FROM METHANOL OVER OXIDE CATALYST

1972 - Russia
1982 - Czech Republic, Bulgaria

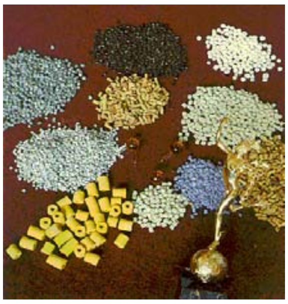
DEHYDROGENATION CATALYSTS FOR ELASTOMERS PRODUCTION

1974 - Russia



TECHNOLOGY OF ALUMINA PRODUCTION: NITRATE-AMMONIA TECHNOLOGY, THERMAL DECOMPOSITION WITH THE USE OF CHG, THERMOCHEMICAL AND MECHANOCHEMICAL ACTIVATION

1975 - Germany, 1990 - Kazakhstan,
1992 - Russia



CATALYSTS FOR PROPYLENE POLYMERIZATION

1980 - Kazakhstan, 1987 - Russia
1995 - The Netherlands, USA

CATALYST FOR NITROUS GASES PURIFICATION FROM OXYGEN IN HYDROXYLAMINE SULFATE PRODUCTION

1981 - Russia, 1995 - Germany

TECHNOLOGIES AND REACTORS BASED ON REVERSE-PROCESS

1982 - Russia, 1985 - Kazakhstan,
1989 - Japan, 1990 - Bulgaria,
1991 - Uzbekistan, 1993 - China,
1995 - USA, 1998 - Australia

CATALYTIC HEATING PLANTS

1982 - Russia

NEW CARBON MATERIAL - SIBUNIT AND SIBUNIT BASED CATALYSTS

1984 - Russia

CATALYSTS FOR METHIONINE PRODUCTION

1986 - Russia

“ZEOFORMING” PROCESS FOR THE PRODUCTION OF HIGH-OCTANE GASOLINES (BIC - SEC “ZEOSIT)

1992 - Russia, 1997 - Poland

NONPLATINUM HONEYCOMB CATALYSTS TO PRODUCE NITRIC ACID

1995 - Russia

CATALYSTS FOR CLAUS PROCESS

1996 - France

Industrial Reverse-Plant for processing of waste gases of metallurgy to H_2SO_4. Capacity up to 100 000 m^3/h ("Pechenganickel” Metallurgy Plant)

CATALYSTS FOR LOW-TEMPERATURE CONVERSION OF CARBON MONOXIDE IN AMMONIA PRODUCTION

1996 - Kazakhstan

Reactor for ammonia oxidation with IC-42-1 catalyst (AO “Azot”, Berezniki)

DEVELOPMENTS OF THE BORESKOV INSTITUTE OF CATALYSIS AT SEMI-COMMERCIAL SCALE

TECHNOLOGIES BASED ON "CATALYTIC HEAT GENERATORS" - COMBUSTION, DRYING AND THERMAL TREATMENT

1984 - Russia, Ukraine, Lithuania

DEVICES AND INSTALLATIONS FOR CATALYSTS TESTING

1985 - Russia, 1992 - USA

ENVIRONMENTALLY FRIENDLY AIR HEATER

1986 - Russia, Uzbekistan

CATALYSTS FOR PLANT OILS HYDROGENATION, PRODUCTION OF MEDICINES (LIDOCAIN, SULPIRID)

1988 - Russia

PROCESSES FOR GASES AND WASTE WATER PURIFICATION FROM SULFUR-CONTAINING SUBSTANCES

1989 - Russia

CATALYIC NEUTRALIZER FOR PURIFICATION OF AUTOMOTIVE EXHAUSTS

1990 - Russia

NOVEL COMPOSITE SORBENTS BASED ON CARBON MATERIALS, ALUMINAS, SILICA GELS FOR WASTE WATER PURIFICATION, PRECIOUS METALS EXTRACTION, FRESH WATER RECOVERY

1995 - Russia

CATALYSTS FOR ACRYLIC ACID PRODUCTION

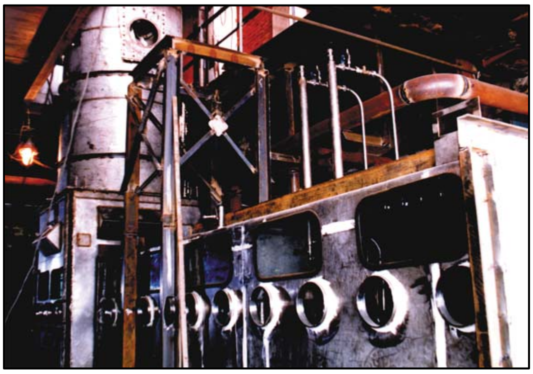
1992- Russia

ALKYLATION OF AROMATICS OVER ZEOLITE CATALYSTS

1990 - Russia

CATALYSTS FOR PRODUCTION OF ULTRA-HIGH MOLECULAR WEIGHT POLYETHYLENE (UHMWPE) AND ETHYLENE-PROPYLENE COPOLYMERS

1997 - Russia



Industrial plant for destruction of mixed organic wastes containing natural uranium with a capacity of 50 t/y (Novosibirsk Chemical Concentrates Plant Ltd.)

Pilot plant for synthesis of phenol from benzene, with nitrous oxide used as the oxidant (ALPHOX, USA)

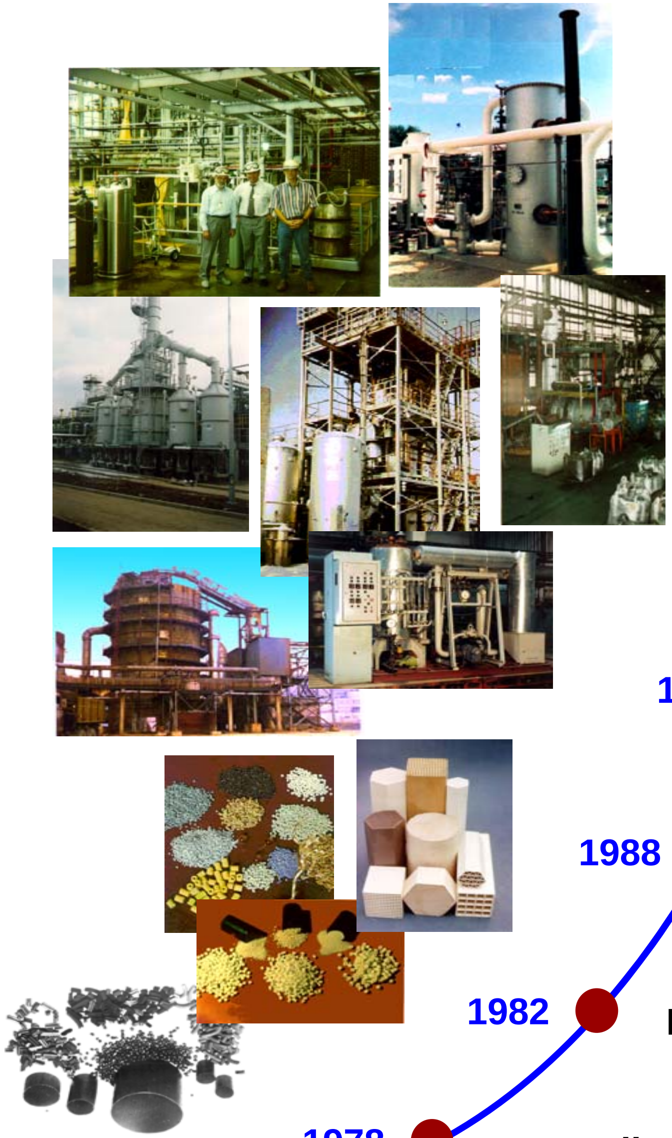
CATALYTIC PROCESS TO DESTRUCT ORGANIC RADIOACTIVE WASTES

1995 - Russia

ONE-STAGE PROCESS OF BENZENE TO PHENOL OXIDATION (ALPHOX)

1996 - USA

Catalytic Processes from Molecular Level to Industrial Plants



1999 Catalyst for hydropurification of terephthalic acid
Developed in cooperation with Samsung Chemicals

1998 One-step technology for production of nicotinic acid
Licensed to European company

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

1996 BtoP technology (benzene + [N_2O] → phenol)
Jointly designed with Monsanto

1995 Catalyst for oil cracking, Russia

1993 Carbon material SIBUNIT, Russia
Sibunit for phosgene synthesis, DuPont, 1994

1992 ZEOFORMING process for synthesis of gasoline, Russia
Lurgi, 1997

1988 Catalysts for polypropylene polymerization, Russia
DSM, 1995

1982 REVERS-Process
Monsanto Enviro Chem. Systems, 1992

1978 Vanadium catalysts for sulfuric acid production, Russia

1958

Kinetic

Gradientless and integral differential reactors
Fast relaxation technique
Stop flow technique
Radiochemical 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*
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.

The Institute of Catalysis invites all researchers interested in collaboration for mutual-benefit cooperation in the field of catalysis.

Long-term visits of foreign specialists to the Boreskov Institute of Catalysis

Canada	3	France	12	The Netherlands	10
Denmark	2	Germany	3	Poland	5
Finland	2	Japan	12	South Korea	1
				USA	15

Long-term visits of the specialists from the Boreskov Institute of Catalysis to foreign institutions

Belgium	2	Germany	25	Norway	2
Bulgaria	5	Greece	3	Poland	5
Canada	1	Hungary	4	Spain	14
China	1	India	1	Sweden	2
Czech Republic	6	Israel	1	Switzerland	2
Denmark	3	Italy	9	UK	5
Finland	2	Japan	5	USA	19
France	6	The Netherlands	9	Yugoslavia	1

SCIENTIFIC COOPERATION WITHIN THE FRAMEWORK OF CONTRACTS AND AGREEMENTS WITH 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,** Messina – **BIC**, Novosibirsk, "*Catalysis for Solving the Energy Problem*".

FRANCE

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

- with the **Institut de Recherches sur la Catalyse**, Villeurbanne on the BIC-IRC Twinning Program:

1. Membranes in Catalysis
2. Studying of Reaction Mechanism of a) Selective Oxidation, b) NO Reduction with Methane in Oxygen Excess over Fiber Glass Materials, c) Monte-Carlo Modelling of Reactions of Selective Oxidation.
3. Studying of Reaction of Hexachloro-Benzene Hydrodechlorination over Pd-Ni, Pd-Cu, Pd-Pt Catalysts
4. Molecular Dynamics in Zeolites;

- with the **Université Pierre et Marie Curie**, Paris.

YUGOSLAVIA

The agreement between **Interacademic Board on Catalysis of the Serbian Academy of Sciences and Arts** and **BIC** in the field of fundamentals of catalyst preparation and catalytic processes.

COOPERATION WITH FOREIGN ORGANIZATIONS IN THE FRAMEWORK OF BILATERAL AGREEMENTS

GERMANY

Cooperation in the frame of RAS-DFG agreement with the **Munich University**, Munich**;** **Munich Technical University**, Garching; **Fritz-Haber-Institut MPG**, Berlin.

COOPERATION IN THE FRAMES OF PROJECTS FINANCED BY INTERNATIONAL FOUNDATIONS

INTAS SUPPORTED PROJECTS

I. Formation and Development of Microporosity in Precursors and Polymer-Pirolysed Activated Carbons with Regards to the Separation Concentration and Storage of Methane

Project Coordinator:

Prof. B. McEnaney, University of Bath, UK.

Participants:

Dr. D. Efremov, Boreskov Institute of Catalysis, Novosibirsk, Russia; **Prof. M. Molina-Sabio**, University of Alicante, Spain; **Dr. A. Bagreev**, Institute of Sorption and Problems of Endoecology, Kiev, Ukraine.

II. Combustion Processes in Porous Media as a Base for New Industrial Technologies

Project Coordinator:

Prof. G. Sivashinskii, Tel-Aviv University, School of Mathematical Sciences, Department of Applied Mathematics, Israel.

Participants:

Prof. A. Noskov, Boreskov Institute of Catalysis, Novosibirsk, Russia; **Prof. V. Babkin**, Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia; **Prof. D. Bradley,** University of Leeds, UK; **Prof. A. Sagindykov**, Combustion Problem Institute, Almaty, Kazakhstan; **Prof. V. Sobolev**, Samara State University, Samara, Russia.

III. Dynamic Behavior of Hydrocarbons in Zeolite Pores

Project Coordinator:

Prof. C.R.A. Catlow, The Royal Institution of Great Britain, London, UK.

Participants:

Dr. A. Shubin, Boreskov Institute of Catalysis, Novosibirsk, Russia; **Dr. H. Jobic**, Institut de Recherches sur la Catalyse, Villeurbanne, France; **Prof. V. Skirda**, Kazan State University, Kazan, Russia.

IV. Electronic, Magnetic and Adsorption Properties of Carbon Nanostructured

Project Coordinator:

Prof. J. Marc-Bonard, Ecole Polytechnique Federale de Lausanne, Switzerland.

Participants:

Dr. V. Kuznetsov, Boreskov Institute of Catalysis, Novosibirsk, Russia; **Prof. O. Klein**, Ecole Polytechnique, Palaiseau, France; **Dr. A. Okotrub**, Institute of Inorganic Chemistry, Novosibirsk, Russia; **Dr. T. Kononenko**, General Physics Institute, Moscow, Russia.

V. Novel Nanostructured Catalysts for the Selective Reduction of NO_x by Heavy Hydrocarbons

Project Coordinator:

Prof. J. Ross, University of Limerick, Ireland.

Participants:

Prof. V. Sadykov, Boreskov Institute of Catalysis, Novosibirsk, Russia; **Prof. A. Rosovskii**, Topchiev Institute of Petrochemical Synthesis, Moscow, Russia; **Prof. V. Matyshak**, Semenov Institute of Chemical Physics, Moscow, Russia; **Prof. B. Andersson**, Chalmers University of Technology, Göteborg, Sweden.

VI. Theoretical and Experimental Studies on the Catalytic Activity of the V_2O_5-TiO_2 System

Project Coordinator:

Prof. K. Jug, Universität of Hannover, Germany.

Participants:

Prof. O. Lapina, Boreskov Institute of Catalysis, Novosibirsk, Russia; **Prof. V. Borovkov**, Institute of Organic Chemistry, Moscow, Russia; **Prof. C. Minot,** Université Pierre et Marie Curie, Paris, France.

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

Project Coordinator:

Prof. 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.

VIII. 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. Niewenhuys, Leiden University, The Netherlands.

Participants:

Prof. N. Jager, University of Bremen, Germany; **Prof. R. Imbihl,** University of Hannover, Germany; **Dr. 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.

IX. Nanocarbons as Building Blocks for New Materials

Project Coordinator:

Prof. H. Kuzmany, University of Vienna, Vienna, Austria.

Participants:

Dr. A. Chuvilin, Dr. V. Kuznetsov, Boreskov Institute of Catalysis, Novosibirsk, Russia.

X. Catalytic Materials

Project Coordinator:

Prof. P. Siffert, EMRS, Strasbourg, France.

Participants:

Prof. Z. Ismagilov, Boreskov Institute of Catalysis, Novosibirsk, Russia; **Dr. R.L. Keiski,** University of OULU, Linnanmaa, Finland; **Prof. J. Santamaria**, University of Zaragoza, Zaragoza, Spain; **Prof. P.G. Menon**, University of Gent, Gent, Belgium.

GRANTS PROVIDED BY INTAS-RFBR

I. Silica and Zirconia Based Mesoporous Mesophases: Synthesis, Structure, and Catalytic Properties

Project Coordinator:

Prof. G. Poncelet, Universite Catholique de Louvain, Belgium.

Participants:

Dr. V. Romannikov, Boreskov Institute of Catalysis, Novosibirsk, Russia; **Prof. F. Schuth**, Universität Frankfurt, Germany; **Prof. S. Kirik,** Institute of Chemistry and Chemical Engineering, Krasnoyarsk, Russia.

II. Study of Microstructure of Free Volume in High Permeability Polymers: Comparison with Microporous Sorbents

Project Coordinator:

Prof. D. Hofmann, GKSS Research Centre, Institute of Chemistry, Teltow, Germany.

Participants:

Prof. O.M. Il'initch, Boreskov Institute of Catalysis, Novosibirsk, Russia.

GRANT PROVIDED BY DUTCH ORGANIZATION FOR SCIENTIFIC RESEARCH (NWO)

Clusters in Zeolite Materials

Project Coordinator:

Prof. R.A. van Santen, Eindhoven University of Technology, Eindhoven, The Netherlands.

Participants:

Prof. G. Zhidomirov, Boreskov Institute of Catalysis, Novosibirsk, Russia; **Prof. V. Kazansky**, Zelinsky Institute of Organic Chemistry, Moscow, Russia.

COPERNICUS

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

Project Coordinator:

Prof. S.G. Neophytides, Institute of Chemical Engineering and High Temperature Chemical Processes Platani Achaias, Greece.

Participants:

Prof. R.M. Ormerod, Kcele University, Staffordshire, UK; **Dr. A. Demin**, Institute of High Temperature Electrochemistry, Ekaterinburg, Russia; **Prof. C. Comninellis**, Swiss Federal Institute of Technology, Lausana, Switzerland; **Prof. V. Sobyanin,** Boreskov Institute of Catalysis, Novosibirsk, Russia; **Prof. V. Khukharov,** University of Chemical Technology and Metallurgy, Sofia, Bulgaria; **Dr. N. Zakharina**, 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. V. Kirillov, Acad. V. Parmon, Prof. T. Yurieva, 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. Dr.-Ing. 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**, Group of the University of Czestochowa, Czestochowa, Poland; **Prof. K. Warmuzinski**, Institute of Chemical Engineering of the Polish Academy of Sciences, Gliwice, Poland; **Prof. P. Forzatti**, Research Group at Department of Industrial Chemistry and Chemical Engineering “Natta” at Politecnico di Milano, Milano, Italy.

IV. Wood Biomass and Wastes Upgrading: Development and Application of Clean Processes for Fine Chemicals, Oils and Carbon Sorbents Production

Project Coordinator:

Prof. R. Gruber, University of Metz, Metz, France.

Participating Institutions:

Boreskov Institute of Catalysis, Novosibirsk, Russia **(Prof. A. Startsev), Krasnoyarsk Institute of Chemistry**, Krasnoyarsk, Russia; **Paris VI University**, Paris, France**; Universitaire de Technologie de Metz**, Metz, France; **Nancy University**, Nancy, France; **Orléans University**, New Orleans, France; **Bruxelles University**, Brussels, Belgium; **Imperial College,** University of London, London, UK; **CSIC Institute of Carbochemistry**, Zaragoza, Spain; **Kassel University**, Kassel, Germany; **Krasnoyarsk Technological Academy,** Krasnoyarsk, Russia; **Donetsk Institute of Coal Chemistry NAU**, Donetsk, Ukraine; **Warszawa Institute of Organic Chemistry PAN**, Warszawa, Poland; **Gliwice Institute of Coal Chemistry**, Gliwice, Poland.

V. Rational Design of Novel Monolithic Materials for the Combined Desulfurization/Denitrogenation of Hot Coal Gases

Project Coordinator:

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

Participants:

Prof. Z. Ismagilov, Boreskov Institute of Catalysis, Novosibirsk, Russia; **Prof. B. Radomysky**, Institute of Chemistry and Technology of Petroleum and Coal, Wroclaw, Poland; **Dr. H. Spliethoff**, Institute for Process Engineering and Power Plant Technology, Stuttgart, Germany; **Prof. Yu. Plyuto**, Institute of Metal Physics, Kiev, Ukraine.

NATO: SCIENCE FOR PEACE PROGRAM

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.

II. Development of Shape Steam Reforming Catalysts

NATO Country Project Director:

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

Partner Country Project Director:

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

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:

Prof. E. Savinov, Boreskov Institute of Catalysis, Novosibirsk, Russia.

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

NATO Country Project Director:

Prof. T. Blasco, Instituto de Tecnologia Quimica, Valencia, Spain.

Partner Country Project Co-Director:

Prof. A. Startsev, Boreskov Institute of Catalysis, Novosibirsk, Russia.

NATO SCIENCE PROGRAMME

Cooperative Science & Technology Sub-Programme

Mechanism of Donor Molecules Activation over the Sulfide Hydrotreating

NATO Country Project Director:

Dr. M. Lacroix, Institut de Recherches sur la Catalyse, Villeurbanne, France.

Partner Country Project Director:

Prof. A. Startsev, Boreskov Institute of Catalysis, Novosibirsk, Russia.

INTERNATIONAL SCIENCE AND TECHNOLOGY CENTER (ISTC)

I. Development of Technology of Catalytic Fluidized Bed Destruction of Mixed Liquid Organic Wastes from Radio-Chemical and Chemical Metallurgy Plants

Project Manager:

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

Participating Institutions:

Pacific Northwest National Laboratory, USA; **Lawrence Livermore National Laboratory**, USA; **Siberian Chemical Complex**, Seversk, Russia; **Novosibirsk Chemical Concentrates Plant Ltd.,** Novosibirsk, Russia; **Novosibirsk State Design-Exploratory Institute VNIPIET**, Novosibirsk, Russia.

II. Development of Technology of Catalytic Fluidized Bed Destruction of Components of Rocket Fuels

Project Manager:

Dr. M. Kerzhentsev, Boreskov Institute of Catalysis, Novosibirsk, Russia.

Project Scientific Leader:

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

Participating Institutions:

Netherlands Energy Research Foundation, The Netherlands; **LERCSI Laboratory**, Louis Pasteur University, France; **State Rocket Center's Makeyev Design Bureau**, Miass, Russia; **Novosibirsk State Design-Exploratory Institute VNIPIET**, Novosibirsk, Russia; **Russian Applied Chemistry Research Center**, St. Petersburg, Russia; **Federal Research & Production Corporation "Altai"**, Biisk, Russia.

III. Creation of Ecological Autonomous Domestic Unit Heater of 25-50 kW Capacity, Based on Catalytic Oxidation of Gaseous Hydrocarbon Fuel

Project Coordinator:

Prof. Valerii A. Kirillov, Boreskov Institute of Catalysis, Novosibirsk, Russia.

CONFERENCE AND EXHIBITION ACTIVITIES

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.

EXHIBITION ACTIVITY

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.

In 2000, the most important BIC's achievements in the area of applied catalysis were presented at the exhibitions:

- *3rd International Exhibition "Innovations-2000. New Materials and Chemical Products",* 11-14 April, Moscow, Russia - **Diploma** for the developments "Synthetic Carbon Sorbents of "Sibunit" Type" and "Catalytic Heat-Extraction Plants";
- *28th International Salon of Inventions, Novel Technique and Wares*, 12-16 April, Geneva, Switzerland – **Diploma and Golden Medal** for REVERSE-process;
- *"ACHEMA-2000",* 22-27 May, Frankfurt-am-Main, Germany;
- "*High Technologies. Investments. Innovations", "Hi-Tech 2000",* 13-16 June, St. Petersburg, Russia – **Diploma** for Catalytic Gas Heaters;
- *9th International Specialized Exhibition "SpasSib-2000»*, 12-14 September, Novosibirsk, Russia – **Big Golden Medal** for "Sulfacrilate" and Diploma for Photocatalytic Air Cleaner;
- *International Fair "HI TECH",* 11-17 October, ShenZhen, China;

- *4th International Exhibition "Science. Scientific Devices*", 16-20 October, Moscow, Russia – **Diploma** for participation;
- *"Science of Siberia – 2000",* 24-27 October, Novosibirsk, Russia – **Minor Golden Medal** for "Sibunit" and **Diploma** for "Selective Water Sorbents";
- *"Russian Medical Technique",* 1-3 November, Novosibirsk, Russia;
- *Exhibition within the framework of the VI Conference "Analytics of Siberia and Far East",* 21-24 November, Novosibirsk, Russia;
- *"Golden Innovations of Russia and CIS Countries",* 6-9 December, Moscow, Russia.

The most attractive were the developments suggested for social fields such as medicine, heat power engineering, food industry and environmental protection. The high scientific and engineering level of developments of our Institute, the manner of presenting them at the exhibitions is always attractive to numerous visitors (including journalists).

CONFERENCE ACTIVITY

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 researchers from CIS, but International as well.

Yu.I. Yermakov Memorial Seminar
"New Approaches to Intentional Synthesis and Characterization of Catalysts"

Novosibirsk, Russia, 6-8 June, 2000

The Conference was devoted to the memory of Professor Yu.I. Yermakov and scheduled to his 65th anniversary. It took place at the Conference Hall of the Boreskov Institute of Catalysis.

The Conference was organized by:

- Boreskov Institute of Catalysis, Novosibirsk, Russia
- Omsk Department of the Boreskov Institute of Catalysis, Omsk, Russia

73 participants - Yu. Yermakov colleagues and followers form our country as well as from France, Germany and Hungary have gathered in Novosibirsk.

The Scientific Program of the Conference comprised 4 plenary lectures, 16 invited lectures, 20 oral presentations and 34 posters.

Plenary lectures were given by**:**

J.M. Basset, Laboratory of Surface OrganoMetallic Chemistry, Villeurbanne, France - "*Recent Aspects of Surface Organometallic Chemistry"*

V.A. Likholobov, Boreskov Institute of Catalysis, Novosibirsk - *"Purposeful Synthesis Ideology for Catalytic Systems Meant to Solve Problems of Small Scale Production of Organic Compounds"*

V.A. Zakharov, Boreskov Institute of Catalysis, Novosibirsk – **“***Methylalumoxane (MAO) Structure and Active Sites Generation in Catalytic Systems Zirconocenes/MAO”*

L. Guczi, Institute of Isotope and Surface Chemistry, Chemical Research Center, Budapest, Hungary – “*Structure and Activity: Gold Nanoparticles Prepared by Coprecipitation and Pulsed Laser Deposition”*

Invited lectures:

F.K. Shmidt, L.B. Belykh, T.V. Cherenkova **(**Irkutsk State University, Irkutsk) – “*Microheterogeneous Catalysts Based on Palladium Complexes: Synthesis and Nature”*

G.V. Lisichkin (Moscow Lomonosov State University, Moscow) – “*Functional Supports with a Patch Structure of Graft Coat”*

S.P. Gubin (Kurnakov Institute of General and Inorganic Chemistry, Moscow) – “*Metal Containing Nano Particles in Polymer Matrices: Synthesis, Structure, Properties*”

B.V. Romanovskii (Moscow Lomonosov State University, Moscow) – “*Nanostructures Based on Molecular Sieves”*

A.A. Galkin, B.G. Kostiuk, N.N. Kuznetsova, M. Polyakov*, A.O. Turakulova, V.V. Lunin (Moscow Lomonosov State University, Moscow; *Nottinham University, Chemical Department, UK) – “*New Technologies to Prepare Heterogeneous Catalysts and Supports Using Water in Subcritical and Over Critical State”*

G.P. Belov (Institute of Chemical Physics, Chernogolovka) – “*Functional Copolymers Based on Vinyl Monomers and Carbon Monoxide”*

L.A. Novokshonova, N.Yu. Kovaleva, I.N. Meshkova, T.M. Ushakova, Yu.A. Gavrilov, V.G. Krasheninnikov, T.A. Ladygina, I.O. Leipunskii*, A.N. Zhigach*, M.L. Kuskov* (Semenov Institute of Chemical Physics, Moscow; *Institute of Energy Problems of Chemical Physics, Moscow) – “*Heterogenization of Metal Organic Catalysts and Analysis of Active Sites Heterogeneity*”

N.M. Bravaya, A.N. Panin (Institute of Chemical Physics, Chernogolovka) – “*Trimary Catalytic Systems Based on Metallocene Complexes, Triisobutyl Aluminum, Perfluoroborates in Ethylene Polymerization”*

G.D. Bukatov, V.A. Zakharov **(**Boreskov Institute of Catalysis, Novosibirsk) – “*Propylene Polymerization on Ziegler-Natta Catalysts: Number and Growth Rate Constant for Stereo Specific and Non Specific Sites”*

V.I. Tsvetkova, P.M. Nedorezova, A.M. Aladyshev, D.V. Savinov, A.N. Klyamkina, D.A. Lemenovskii* (Semenov Institute of Chemical Physics, Moscow, *Moscow Lomonosov State University, Moscow) – “*Bulk Propylene Polymerization over Metallocene Catalyst. Influence of Catalyst Composition and Structure on System Activity, and Polypropylene Microsctructure and Properties”*

V.K. Duplyakin (Omsk Department of the Boreskov Institute of Catalysis, Omsk) – "*Design of Supported Catalytic Systems*"

B.N. Kuznetsov, N.V. Chesnokov, N.M. Mikova, L.V. Naimushina (Institute of Chemistry and Chemical Engineering, Krasnoyarsk) – "*Metal Carbonyls for Preparing Supported Catalysts for Reactions Involving Carbon Monoxide*"

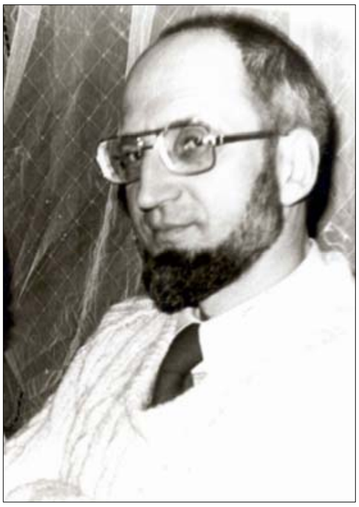
A.N. Startsev (Boreskov Institute of Catalysis, Novosibirsk) – "*Molecular Mechanism of Catalysis by Sulfide Catalysts for Deep Hydrotreatment of Oil Fractions*"

V.I. Smetaniuk (Topchiev Institute of Petrochemical Synthesis, Moscow) – "*Similarity and Difference Between Homogeneous and Gel-Immobilized Metallocomplex Catalytic Systems*"

A.A. Efendiev, L.S. Molochnikov*, S.Yu. Menshikov** (Azerbaidjan Institute of Polymer Materials AAN, Sumgait, *Ural State Forestry Academy, Ekaterinburg, **Ural Institute of Organic Synthesis, Ekaterinburg) – "*Metallopolymer Complex Catalysts with Memory*"

A.A. Dulov, L.A. Abramova, S.P. Baranov*, A.A. Uelskii** (Zelinskii Institute of Organic Chemistry, Moscow, *Lebedev Institute of Physics, Moscow, **State Research Center «Institute of Chemistry and Chemical Engineering of Element Organic Compounds», Moscow) – "*Modeling of Metal Nanoclusters Forming at CVD-Synthesis of Catalysts*"

V.B. Shur, S.M. Yunusov (Nesmeyanov Institute of Element Organic Compounds, Moscow) – "*Towards Catalysts for Low Temperature Ammonia Synthesis: Results and Perspectives*".



Yu.I. Yermakov took an active part in formation of the Institute. In 1963 he became the Head of the Laboratory of Catalytic Polymerization, in 1972 - the Head of the Department of Homogeneous and Coordination Catalysis. Yu.I. Yermakov was the founder of new direction in heterogeneous catalysis – catalysis by anchored metal complexes, the main idea of which was purposeful synthesis of anchored organometallic, cluster and metal catalysts. Yu.I. Yermakov studied in detail mechanism of selective oxidation and olefin carbonylation. He put forward an idea about new porous carbon material "Sibunit" widely used now for production of adsorbents and supported catalysts. Yu.I. Yermakov suggested an original approach to synthesis of catalysts for olefin polymerization.

We remember him as an extraordinary organizer, talented scientist and a very interesting person.

V.V. Popovskii Memorial Seminar "Regularities of Deep Catalytic Oxidation"

Novosibirsk, Russia, 22 May, 2000

The Seminar devoted to the memory of Professor V.V. Popovskii and scheduled to his 70th anniversary took place at the Conference Hall of the Boreskov Institute of Catalysis.

76 scientists attended the Seminar. The scientific program of the Seminar included 6 plenary lectures and 28 poster presentations.

Plenary lectures were presented by:

N.N. Bulgakov, V.A. Sazonov (Boreskov Institute of Catalysis, Novosibirsk) – "*Catalysts for Combustion. Bonding Strength of Oxygen*"

Z.R. Ismagilov (Boreskov Institute of Catalysis, Novosibirsk) – "*Reactivity of Organic Compounds in Deep Catalytic Oxidation*"

V.S. Muzykantov (Boreskov Institute of Catalysis, Novosibirsk) – "*From Isotope Exchange of Oxygen to Isotopic Kinetics*"

Yu.M. Staroseltsev, S.A. Yashnik, A.P. Vityugov, Z.R. Ismagilov, N.M. Danchenko* (Boreskov Institute of Catalysis, Novosibirsk; *Motor-Transport Neutralizers Factory, Novouralsk) – *"Ecological Problems of Motor Transport and Methods of their Solution"*

N.M. Popova (Institute of Organic Catalysis and Electrochemistry, Almaty, Kazakh Republic) – *"Physico-Chemical Foundations for Synthesis of Supported Metal and Oxide Catalysts for Gas Purification"*

Yu.V. Ostrovskii, G.M. Zabortsev, A.A. Shpak, Z.R. Ismagilov*, V.A. Sazonov*, V.D. Meshcheryakov (Exploratory Design Institute VNIPIET, Novosibirsk; *Boreskov Institute of Catalysis, Novosibirsk) – "*Catalytic Oxidation of Organic-Compounds Vapours in Off-Gases*"

Professor Vladislav V. Popovskii was one of the first collaborators of the Institute and did much for its organization being the first Scientific Secretary.

He made an important contribution to the development of scientific concept of the nature of catalytic action, to origination of new actual direction – application of catalysis to environmental protection. V. Popovskii carried out a wide range of systematic investigations of catalysts and oxidized substances, and revealed the determinative role of oxygen bond strength for oxidation processes.

V. Popovskii developed a series of efficient catalysts and technologies for industrial waste detoxification.

He was an outstanding teacher, the main lecturer at the Department of Catalysis and Adsorption of the Novosibirsk State University and many of his disciples became leading scientists of the Boreskov Institute of Catalysis and other institutes.

All his friends remember V. Popovskii as a very energy, cheery fellow and inventor.

IV Russian Conference with the Participation of CIS Countries "Scientific Fundamentals of Catalyst Preparation and Technology" and III Russian Conference with the Participation of CIS Countries "Problems of Catalysts Deactivation"

Sterlitamak, Bashkortostan, 29 August-1 September, 2000

The Conference was organized by

- Bashkortostan Academy of Sciences, Ufa
- Institute of Petroleum Chemistry and Catalysis of the Academy of Sciences of Bashkortostan and USC RAS, Ufa
- Republican Government, Ufa
- Boreskov Institute of Catalysis, Novosibirsk
- Russian Foundation for Basic Research (RFBR)
- Ministry of Industry, Science and Technology of Russian Federation, Moscow
- The Russian Scientific Council on Catalysis, Moscow
- JSC "Kaustik", Sterlitamak

Two representative Scientific and Practical Conferences (two in one), i.e. the 4th Conference "Scientific Fundamentals of Catalysts Preparation and Technology" and the 3rd Conference "Problems of Catalysts Deactivation" took place at Sterlitamak City that is one of the large chemical and petrochemical centers of Republic Bashkortostan, where the "islands" of the catalyst industry are still kept.

The total number of participants of two Conferences was 140. The Conferences Programs included 20 plenary lectures and 87 oral presentations.

Plenary lectures:

A.L. Lapidus, I.G. Solomonic, A.Yu. Krylova, E.G. Krasheninnikov* (N.D. Zelinskii Institute of Organic Chemistry, Moscow; *RSC "Kurchatov Institute", Moscow) – *"Effect of Plasma Afterglow on Cobalt Catalysts Formation"*

G.R. Kotel'nikov (JSC "YARSINTEZ", Yaroslavl) – *"Problems of Manufacturing and Lifetime of the Catalysts for Petrochemistry*"

M.I. Levinbuk, M.L. Pavlov* (Russian Gubkin State University of Petroleum and Gas, Moscow; *JSC "Salavatnefteorgsintez", Salavat) - *"Outlook for Domestic Cracking Catalysts Production in Russia"*

A.V. Balaev**, S.I. Spivak (**Institute of Petroleum Chemistry and Catalysis, Ufa) – *"Modelling of Processes over the Catalysts with Variable Properties"*

V.K. Duplyakin (Omsk Division of the Boreskov Institute of Catalysis, Omsk) – *"Commercial Catalysts for Oil Refining and Oil Chemistry. State of Production and Recent Developments"*

A.A. Galkin, M. Polyakov*, V.V. Lunin (Moscow Lomonosov State University, Moscow; *Nottingham University, UK) – *"Synthesis of Oxide Catalysts and Supports in Sub- and Above-Critical Water"*

Yu.G. Shirokov (Ivanovo State Chemical-Technological University, Ivanovo) – *"Redox Reactions upon Mechanochemical Synthesis of Catalysts"*

V.V. Molchanov, R.A. Buyanov (Boreskov Institute of Catalysis, Novosibirsk) – *"Scientific Fundamentals for Application of Mechanochemistry for Catalysts Preparation"*

Z.R. Ismagilov, A.M. Khanov*, E.V. Matygullina*, G.F. Dobrynin** (Boreskov Institute of Catalysis, Novosibirsk; *Institute of Technical Chemistry, Perm; **JSC "KERAMEK", Perm) – *"Monolith Honeycomb Catalysts. Preparation and Production Technology* "

V.A. Sadykov, M.V. Chaikina*, S.N. Pavlova (Boreskov Institute of Catalysis, Novosibirsk; *Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk) – *"Development of Scientific Fundamentals for Synthesis of Highly Dispersed Framework Zirconium Phosphates – Catalysts for Paraffines Isomerization and Selective Oxidation to Olefins"*

V.P. Doronin, T.P. Sorokina **(**Omsk Division of the Boreskov Institute of Catalysis, Omsk) – *"Development and Application of Domestic Microspherical Catalysts for Cracking"*

I.I. Kurlyandskaya, Yu.A. Treger, M.P. Flid ("SINTEZ", Moscow) – *"Novel Trends in Preparation of Catalysts for Chloroorganic Processes"*

E.Z. Golosman (JSC "Novomoscowsk Institute of Nitric Industry", Novomoscowsk) – *"Main Regularities of Synthesis of Cement-Containing Catalysts for Various Processes of Organic, Inorganic and Ecological Catalysis"*

A.S. Ivanova (Boreskov Institute of Catalysis, Novosibirsk) – *"Fine Zr-Based Oxide Systems: Synthesis, Properties and Application"*

U.M. Dzhemilev (Institute of Petroleum Chemistry and Catalysis, Ufa) – "*Metal Complex Catalysts: Novel Chemical Technologies"*

V.I. Smetanyuk, A.V. Ivanyuk (A.V. Topchiev Institute of Petrochemical Synthesis, Moscow) – *"Complex Metal Gel-Immobilized Catalytic Systems – Optimum Catalysts for Liquid Phase Petrochemical Processes"*

E.I. Bagrii, A.V. Avdeev, G.B. Maravin, E.N. Karaulova (A.V. Topchiev Institute of Petrochemical Synthesis, Moscow) - "*Biomimetic Approach to Development of Catalytic Systems for Saturated Hydrocarbon Processing*"

Yu.B. Monakov, Z.M. Sabirov (Institute of Organic Chemistry, Ufa) – *"Connection between Stereospecificity of Lanthanum Catalysts and Active Centers Structure, Diene Structure, Nature of Cocatalyst and Preparation Conditions"*

G.P. Belov (Institute of Problems of Chemical Physics, Chernogolovka) – *"Palladium Complexes – Catalysts for Synthesis of Functional Polymers based on Carbon Monoxide"*

V.I. Tsvetkova, P.M. Nedorezova, A.M. Aladyshev, A.N. Klyamkina, D.V. Savinov, E.N. Veksler, G.P. Brusova*, D.A. Lemenovskii* (N.N. Semenov Institute of Chemical Physics, Moscow; *Moscow Lomonosov State University, Moscow) – *"Synthesis of Metallocene Catalysts and their Use in the Processes of Homo- and Copolymerization of α-Olefins"*

The subject of Conferences maximum concerned the results of both fundamental and applied investigations on new methods of catalyst synthesis, design of novel catalytic systems and industrial catalysts on its bases, the nature of the processes leading to the decrease of catalyst activity and selectivity. The Conferences participants considered completely different factors, tendencies and regularities influential in catalyst industry and adopted a Resolution.

The presentations of Boreskov Institute of Catalysis (Novosibirsk), "Condea" (Germany), JSC "United Catalyst Co" (Moscow) and Novokuibushevsk Catalyst Plant took place.

International Seminar "Non-Phosgene Technologies in Organic Catalytic Synthesis"

In the frame of the 9th International Symposium on Heterogeneous Catalysis

Varna, Bulgaria, 20-22 September, 2000

The Seminar was hold in a picturesque place on the Bulgarian coast of the Black Sea – St. Constantine and Helen resort, 8 km of Varna.

Seminar Organizers

- Scientific-Engineering Center "Zeosit" of United Institute of Catalysis, Novosibirsk, Russia
- Boreskov Institute of Catalysis, Novosibirsk, Russia
- Institute of Catalysis, Bulgarian Academy of Sciences, Sofia, Bulgaria.

The scope of the Seminar included fundamentals, process applications and technology development of non-phosgene synthesis.

43 participants from 9 countries (USA, Germany, Japan, Italy, India, Korea, Poland, Bulgaria, Russia), representatives of first-rate world companies (Rohm and Haas Company, USA; The Dow Chemical Company, USA; EniChem, Italy; Bayer AG, Germany; General Electric Corporate R&D, USA; UOP, USA) and academic institutes (Boreskov Institute of Catalysis, Russia; Korea Institute of Science and Technology, Korea; National Chemical Laboratory, India; Institute of Catalysis, Bulgaria) have attended the Seminar.

The Seminar participants presented plenary lectures, oral and poster presentations on the following topics:

- *Direct Synthesis of Diisocyanates from Nitro-Compounds*
- *Catalytic Synthesis of Dialkylcarbonates as Alternatives to Phosgene*
- *Synthesis of Diisocyanates via Interaction of Dialkylcarbonates with Diamines*
- *Non-Phosgene Catalytic Synthesis of Polycarbonates*
- *The Technological Aspects of Purification of Dialkyl-Carbonates, Polycarbonates and Diisocyanates after the Non-Phosgene Catalytic Synthesis*

Plenary presentations:

Y. Ono (Tokyo Institute of Technology, Tokyo, Japan) – *"Catalysis in Synthesis and Reactions of Dimethyl Carbonate"*

K.G. Ione (Scientific-Engineering Center "Zeosit", Novosibirsk, Russia) – *"The Non-Phosgene Synthesis of Diisocyanates and Their Precursors"*

Yu. Dergunov (N. Novgorod State Architectural University, N. Novgorod, Russia) – *"Non-Phosgene Methods for Isocyanates Synthesis"*

V.A. Likholobov (Boreskov Institute of Catalysis, Novosibirsk, Russia) – "*New Opportunities in Synthesis of Intermediates for Polyurethane Materials"*

B.K. Nefedov (Ministry of Science and Technologies, Moscow, Russia) – *"Ways and Manufacturing Techniques of Isocyanates"*

S.V. Lopatkin (Novosibirsk State University, Novosibirsk, Russia) – *"Dimethylcarbonate Synthesis: Influence of Support Nature and Structure on Properties of the Catalytic System"*

Participation in the Seminar made it possible to summarize knowledge on the subject, to discuss general progress in this area and stimulate new ideas.

VI Conference "Analytics of Siberia and Far East"

Novosibirsk, Russia, 21-24 November, 2000

The Conference was sponsored by:

- Russian Foundation for Basic Research, Moscow
- Scientific Council on program " Siberia", Novosibirsk
- INTERTECH Corporation, USA
- N.N. Vorozhtsov Institute of Organic Chemistry, Novosibirsk
- Institute of Petroleum Geology, Novosibirsk
- Technological Design Institute of Instrument Engineering for Geophysics and Ecology of SB RAS, Novosibirsk
- Boreskov Institute of Catalysis, Novosibirsk

250 specialists from 30 cities and 3 countries (Germany, Russia, Kazakhstan) participated in the Conference. They presented 20 plenary lectures, 50 oral presentations and 162 posters.

The Scientific Program of the Conference opened the various problems of modern analytical chemistry.

Plenary lectures were given by:

Yu.A. Zolotov (Kurnakov Institute of General and Inorganic Chemistry, Moscow) – *"Analytic Chemistry on the Eve of XXI Century"*

G.I. Baram (Limnological Institute, Irkutsk) – "*High-Efficient Liquid Chromatography and Environmental Monitoring"*

B.G. Derendyaev, V.N. Piottukh-Peletskii (N.N. Vorozhtsov Institute of Organic Chemistry, Novosibirsk) – *"Databases "Molecular Spectrum - Fragment Composition of Compounds " for Analytic IR Spectroscopy and Mass-Spectroscopy"*

V.I. Vershinin, N.B. Il'icheva, I.I. Medvedovskaya, O.V. Sokolova, V.A. Topchii (Omsk State University, Omsk) – "*Reliability of Chromatographic Identification: Criteria Choice"*

V.N. Sidel'nikov, Yu.V. Patrushev (Boreskov Institute of Catalysis, Novosibirsk) – *"Separation Process Acceleration in Gas-Liquid Chromatography"*

A.A. Pupyshev (Ural State Technical University, Ekaterinburg) – "*Study and Prediction of Thermal Chemical Processes in Modern Spectral Sources with the Use of Equilibrium Thermodynamics"*

T.N. Shekhovtsova, N.A. Bagirova, I.A. Veselova, L.E. Grishina, S.V. Muginova, I.F. Dolmanova (Moscow Lomonosov State University, Moscow) – *"New Approaches to Fermentative Methods of Analysis"*

L.I. Pleskach, G.D. Chirkova (Al-Farabi Kazakh State National University, Almaty, Kazakhstan) – *"Advantage of Ultrasonic Intensification of "On-Line" Samples Dissolution"*

V.V. Malakhov, A.A. Vlasov, N.N. Boldyreva, L.S. Dovlitova (Boreskov Institute of Catalysis, Novosibirsk) – *“Novel Aspects of Standard-Free Stoichiography Methods for Chemical Analysis*”

A.G. Tereshchenko, **O.V. Tereshchenko**, V.V. Sokolov, R.Sh. Yunusov (Research Institute of High Voltage at Tomsk Polytechnical University, Tomsk) – *“Software for Analytic Laboratories of Industrial Enterprises”*

L.L. Petrov (Institute of Geochemistry, Irkutsk) – “*Reliability of Analytic Information in Geochemistry upon Using of Standards”*

Yu.S. Shafrinskii, **S.S. Bednarzhevskii** (Institute of Non-Linear Investigations, Novosibirsk) - *“Standards for Estimations of Quality and Safety of Farm Products”*

S.B. Shubina, M.E. Trofimova, T.A. Mel’nichuk, A.A. Bal’chugov (JSC “Ural Metal Institute, Ekaterinburg) – *“The Standards for Detection of Gases in Metals”*

D.G. Lisienko, **M.A. Dombrovskaya**, V.N. Muzgin (Ural State Technological University, Ekaterinburg) – *“Experience in Development and Application of Purity Reagents Standards”*

A.I. Saprykin, G.N. Anoshin* (Institute of Inorganic Chemistry, Novosibirsk; *United Institute of Geology, Geophysics and Mineralogy, Novosibirsk) – *“High Resolution Mass Spectrometry with the Inductively Coupled Plasma and Laser Ablation for Analysis of Geological and Natural Objects”*

V.M. Gruznov, V.G. Filonenko, A.T. Shishmarev (Design-Technological Institute of Geophysical and Ecological Instrument-Making, Novosibirsk) – *“High-Speed Gas Chromatography”*

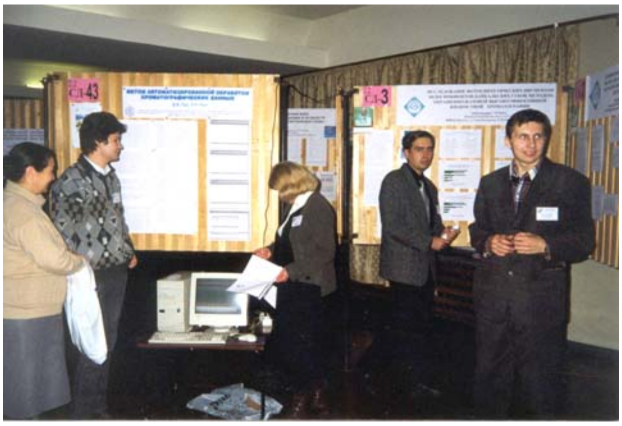
E.A. Kruglov (Bashkirian Scientific-Research Ecological Center, Ufa, Bashkortostan) – *“Adequacy of Analysis of Persistent Organic Pollutants in Food, Natural Feedstock and Environmental Objects”*

V.P. Fadeeva, O.N. Nikulicheva, V.D. Tikhova (Novosibirsk Institute of Organic Chemistry, Novosibirsk) – “*Thermoanalytical Method for Organic Substances Investigation*”

V.I. Fedotov, Yu.P. Meshalkin (Institute of Laser Physics, Novosibirsk; Novosibirsk State-Technological University, Novosibirsk) - *“Laser-Induced Ultra-Violet Fluorescence”*

O.V. Shuvaeva (Novosibirsk Institute of Organic Chemistry, Novosibirsk) – *“Detection of Chemical Mode of Elements by High-Efficient Liquid Chromatography”*

A.A. Zirka, L.N. Shabanova (JSC “Institute of Hydrometallurgy of Non-Ferrous Metals”, Novosibirsk) – “*Software for Metrological Data Processing of the Results of Quantitative Chemical Analysis*”.



The Poster Session was subdivided to 6 Sections:

- Methods of Chromatography and Sorption
- Electrochemical Methods
- Spectral Methods
- Chemical and Physico-Chemical Methods
- Analytical Methods in Biology, Medicine, Pharmacology
- Analysis of Environmental Objects

The following companies: Shimadzu GmbH, Germany; PerkinElmer Instruments, USA; INTERTECH Corporation, USA; Varian Inc., USA; Ural Office of LECO; Russian Companies “Intetrlab”, VMK, “Bioline” gave presentation lectures about new developments.

18 companies took part in the Exhibition of analytic equipment.

BORESKOV INSTITUTE OF CATALYSIS AS AN EDUCATIONAL CENTER

With deep belief that people are a decisive factor and the best way to study yourself is to teach others, many researchers of the Institute participate in the training of specialists in chemistry and, of course, in catalysis. The majority of them ensure closest and time-tested links of the Institute with the main source of researchers – Novosibirsk State University (NSU). The others develop dynamic contacts with other Siberian schools, primarily, with Novosibirsk State Technical University (NSTU).

BIC – NSU

The year 1999, Novosibirsk State University commemorates its 40th anniversary.

Novosibirsk State University was established as an essential part of the Siberian Branch of the Academy of Sciences; at present it embodies the idea of the close integration of education and science. The chief mission of the University is to train professionals for scientific institutions of the country.

From its earliest age, the University pursues *three fundamental principles.* The *first* one is that the teachers are experts engaged in the real science. The intellectual basis of the University is more than 5000 scientists of 30 research institutes of the Siberian Branch. The *second* principle is a thorough mathematical background provided to students of all the departments. The University was among pioneers of application of computer facilities and up-to-date information technologies for students’ training and research. And the *third* principle means that the students master theoretical disciplines during their first to third years and do their practical research in academic institutes of the Siberian Branch during the last years.

Boreskov Institute of Catalysis is a key element in the training of specialists in chemistry at NSU. More than 35 researchers of the Institute are currently part-time teachers at the Department of Natural Sciences (DNS) at NSU. They present lectures, give seminars and practical classes, participate in the organization and renovation of the educational process at four out of eight chemical chairs of DNS, namely, chairs of physical chemistry, general chemistry, analytical chemistry, adsorption and catalysis.

The chair of adsorption and catalysis is of special importance for the Institute. It is only 5 years younger than Novosibirsk State University itself. The organization of the chair was initiated in 1964 by Academician G.K. Boreskov – the founder and first director of the Boreskov Institute of Catalysis SB RAS. The chair is located at the Institute, which provides it with everything required for efficient training of students specializing in catalysis and technology of catalytic processes. Twenty five to thirty students of the IV, V and VI years of the Chemical Department of DNS are trained at the chair annually. Its graduates obtain Bachelors, Specialists and Masters diplomas. Graduation works of the students are conducted at the laboratories of the Institute and are supervised by experienced researchers. Their results are usually published in scientific journals and form the basis of their future Ph.D. theses.

From the first years, the strategy of the training of students at the chair is formed by leading scientists of BIC and harmonically combines two aspects. On the one hand, curricula provide the students with deep theoretical and practical knowledge in catalysis, theory of the prevision of the catalytic action of substances, kinetics of catalytic reactions, scientific bases of the preparation of catalysts, bases of the technology of catalytic processes, application of modern physical and mathematical methods for investigation of catalysts and catalysis. On the other hand, the curricula allow for a significant widening of the sphere of the working activity of its graduates. They can work as technologists, production managers, researchers at various research organizations, teach at universities.

All this allows the students to prepare their graduation study at the highest scientific level and become widely informed specialists in chemistry and catalysis. The graduates of the chair of adsorption and catalysis are the principal source of recruitment of the personnel of the Institute.

BIC – NSTU

Training of the personnel in the field of technology of catalytic processes is of special importance for practical application of fundamental knowledge in the field of catalysis. To meet this task, work in two main directions is under way. First, corresponding courses ("Bases of chemical technology", "Mathematical modeling of catalytic reactors") are prepared for students studying at the chair of adsorption and catalysis. Further progress in this direction is connected with the training of students specializing in "Engineering environment protection" started at NSTU in 1998. It is one of the steps in realization of the program of joint training of specialists at NSTU and institutes of the Siberian Branch of RAS. The basic training is conducted by a chair founded at the Boreskov Institute of Catalysis. Researchers of BIC present courses on industrial ecology and technology of the environment protection, basics of manufacturing and catalytic methods.

BIC – graduate school

Besides teaching students of a number of Russian universities, researchers of the Institute participate in the training of young scientists of the highest qualification capable of independent fundamental, search and applied studies in the field of catalysis. Their training has priority importance for the Institute and is directly related to its development and well being. The Institute solves these problems through the graduate school of SB RAS and graduate school of NSU. Annually 20-30 graduates are trained at the graduate school working at the Institute. Supervised by the researchers of the Institute, graduate students conduct their Ph.D. studies in chemical kinetics and catalysis, physical chemistry, chemical engineering in the BIC laboratories.

There is a great demand for specialists in catalysis trained at the Boreskov Institute of Catalysis, both graduates of the chair of adsorption and catalysis and of the graduate school. Many of them apply their knowledge in these fields at various research centers, universities and manufacturing companies.

SCIENTIFIC SOCIAL LIFE

February, 8, marks the Day of Russian Science. This date (instead of the previous one) has been established by the Presidential Decree of June 7, 1999 in order "to follow the historical traditions and in celebration of 275th anniversary of the creation of the Russian Academy of Sciences ." It was February 8, when Peter the First has signed the Decree of the foundation of the Academy of Sciences.

☆

In the middle of March the Conference of the Novosibirsk Branch of the D.I. Mendeleev Russian Chemical Society has been held at the G.K. Boreskov Institute of Catalysis of the SB RAS. The NB RCS Chairman, Academician Valentin Parmon has opened the Conference. The main problem of the agenda was the problem of training of the young specialists in the field of chemistry in the Novosibirsk Region.

☆

On the 21st of April at the Annual General Meeting of SB RAS the Deputy Director of the Boreskov Institute of Catalysis, Prof. Vladimir Likholobov, was elected the President of Omsk Scientific Center.

☆

July. Two days at the Boreskov Institute of Catalysis the State Examining Board worked. The graduate students of the Engineering Problems of Ecology sub-faculty of the Novosibirsk State Technical University (NSTU) defended their graduation theses. The Academic Chair of the NSTU turned out the first graduation of engineers–ecologists having the specialty "Engineering Protection of Environment".

Prof. A. Noskov, Deputy Director of the Institute, Head of the Chair said: "There is essential distinction in kind between these specialists and graduates from Novosibirsk State University.

The graduate students of the Engineering Problems of Ecology sub-faculty have capacity for technical way of thinking, engineering approach to solving the problems of industrial enterprises. The representatives of chemical institutes and enterprises, who attended the defense, made several interesting propositions. Besides, establishing of the Chair has stimulated the creation of Educational Center in the Institute including computer school".

☆

November, 17, at the House of Scientists of the Novosibirsk Academgorodok under the Russian President V. Putin chairmanship the Regional Conference on the State Strategy of the Siberian Region Development has been held. The chiefs of Republics and Regions included in the structure of the Siberian Federal District, members of the Russian Government, chiefs of departments, heads of large companies and enterprises, leading scientists of Siberia have participated in its work.

☆

November, 19, the great son of Russian people, Academician Michail Alekseevich Lavrentiev was 100. He has lived long and vigorous life of the main enthusiastic creator of the new scientific center at the East of our Country. He has not lived a month up to his 80th anniversary. Michail Alekseevich Lavrentiev was the person of a huge scientific and civil scale for everyone, who knew him. The image of this bright person is indelible. The name of Academician Michail Alekseevich Lavrentiev, outstanding mathematician and mechanician, organizer of science and of youth education, is widely known both in our country and abroad.

☆

The German-Siberian Conference on Economic and Technological Cooperation took place in Novosibirsk on September 24-26. The members of German delegation as well as Russian representatives of the German corporations visited the Boreskov Institute of Catalysis. At the Business Center of the Institute the Director of the Institute Academician Valentin Parmon told the visitors about multifaceted activity of collective headed by him.

An excursion to the Department of Physico-Chemical Methods of Investigation was organized. Dr. A. Boronin stated the opportunities and advantages of the method of Electron Spectroscopy for chemical analysis, and Prof. E. Talsi told about application of NMR method in 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 «Altai», Biisk

- «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. During November 1997 - January 2001 Zamaraev International Charitable Scientific Foundation conducted 7 competitions between young Russian scientists working in the field of chemical catalysis and physical chemistry. The results of these competitions had been summed up, 30 winners received Zamaraev post-graduate scholarships, 20 scholars – student scholarships. These scholarships will help to support young scientists in their researching work.

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.

☆

In October, 1999, after a long interruption, the **Council of Scientific Youth** began to work. At present 9 Ph.D. students and scientific employees of the Institute and also representative of the students form the personnel of the Council. The Chairman of the Council is Dr. A.G. Okunev. 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.

☆

Results of the XXXVIII Annual BIC's Competition of the Research Works

I Prize

V.A. Kirillov, N.A. Kuzin, A.B. Shigarov, A.V. Kulikov, B.N. Luk'yanov, V.D. Meshcheryakov, A.S. Bobrin, V.A. Kuz'min, P.G. Tsyrul'nikov

"Development of Ecologically Sound Self-Contained Heating System with the Capacity 25-50 kWt, Based on Principle of Catalytic Oxidation of Gaseous Hydrocarbon Fuels" (91 points)

II Prizes

A.V. Romanenko, M.N. Timofeeva, E.M. Moroz, V.I. Zaikovskii, I.A. Ovsyannikova, A.V. Golovin

"Catalytic Purification of Terephthalic Acid" (86 points)

K.A. Dubkov, V.I. Sobolev, E.A. Paukshtis, G.I. Ivanov

"Low Temperature Hydrocarbons Oxidation with α-Oxygen" (82 points)

L.Yu. Il'yina, (I.V. Koptyug), Yu.I. Aristov, O.P. Klenov, M.M. Tokarev, N.A. Pakhomov, V.B. Fenelonov

"^{1}H NMR Microimaging Studies *in situ* of the Mass Transport Phenomena in Porous Pellets of Catalysts and Sorbents" (79 points)

V.I. Zheivot, E.M. Moroz, V.I. Zaikovskii, V.Yu. Gavrilov

"Gas Chromatography in Catalytic Studies and Analysis of Natural Objects" (77 points)

III Prizes

M.M. Yulikov, O.N. Mart'yanov, V.F. Yudanov

"Dimensional Effects in Ferromagnetic Spectra" (71 points)

O.N. Baklanova, G.V. Plaksin, V.A. Drozdov, V.Yu. Davydova, T.I. Gulayeva, O.V. Maevskaya

"Synthesis of Microporous Sorbents Based on Vegetable Feedstock" (71 points)

V.N. Romannikov, (S.D. Kirik), V.B. Fenelonov, (L.A. Soloviev), A.N. Shmakov, A.Yu. Derevyankin, (A. Gedeon), N.N. Trukhan, O.B. Lapina, E.A. Paukshtis

"Physico-Chemical Properties of Mesoporous Mesophase Silica Materials, Formed by S^+I^- Mechanism" (70 points)

A.I. Boronin, V.I. Avdeev, S.V. Koshcheev, S.F. Ruzankin, V.F. Malakhov, S.V. Bogdanov, E.M. Moroz, A.N. Salanov, E.A. Ivanov, G.M. Zhidomirov

"High-Temperature Quasimolecular Oxygen Species on the Silver" (69 points)

M.Yu. Smirnov, (G.W. Graham)

"Studies of Pd Oxidation and Reduction in Model $Pd/Ce_{0.7}Zr_{0.3}O_2$ Catalyst"

S.V. Tsybulya, G.N. Kryukova, T.A. Krieger, P.G. Tsyrul'nikov, E.N. Kudrya
"Studies of Structural Transformations in the $MnO_x/\gamma-Al_2O_3$ System upon Thermal Activation" (67 points)

I.V. Mishakov, V.V. Chesnokov, N.A. Pakhomov
"Design of Catalytic Method of Hydrocarbon Chlorderivatives Processing over the Metals of Iron Group" (64 points)

V.N. Panchenko, N.V. Semikolenova, V.A. Zakharov, I.G. Danilova, E.A. Paukshtis
"Study of the Formation of Supported Zirconocene Catalysts for Olefin Polymerization, Obtained with the Use of SiO_2/MAO and SiO_2/ "Borate Activator" Supports" (60 points)

S.Yu. Troitskii, M.A. Fedotov, D.I. Kochubey, B.N. Novgorodov, A.L. Chuvilin
"Polynuclear Hydroxocomplexes Pt(II) and Ru(III) – Precursors of Catalyst Active Component" (58 points).

☆

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. Geogii 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 were 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 Gerogii 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.

BRIEF HISTORY OF THE INSTITUTE, 1979-1988
(a sequel to "Annual Review-98", "Annual Review-99")

In 1988, the Institute of Catalysis celebrated its 30th anniversary. The time has shown that the trends of research initially outlined were properly chosen. The main principle – combination of fundamental and applied research – has proved to be correct. The Institute staff was full of creative ability and energy to do their best in solving the problems of modern science and technique posed by the national economy and the world technical progress.

To the end of 80th the Institute was stuffed by more than 1100 people of whom about 25 Professors and more than 210 had a Ph.D. degree.

Structure of the Institute in the middle of 80th

DEPARTMENT OF HETEROGENEOUS CATALYSIS

Head: Georgii K. Boreskov (up to 1984)

Laboratory of Oxidation	**Head: Academician Georgii K. Boreskov (up to 1984)** **Dr. Alexandr V. Khasin**
Laboratory of Dehydrogenation	**Head: Prof. Roman A. Buyanov**
Laboratory of Metal Catalysts	**Head: Prof. Valerii I. Savchenko**
Laboratory of Zeolite Catalysts	**Head: Prof. Kazimira G. Ione**
Laboratory of Selective Paraffines Conversion	**Head: Prof. Valerii D. Sokolovskii**
Laboratory of Catalysts Preparation	**Head: Prof. Vera A. Dzis'ko**
Laboratory of Catalytic Conversion of Sulfur Compounds	**Head: Prof. Anna V. Mashkina**
Laboratory of Ecological Catalysis	**Head: Prof. Vladislav V. Popovskii**
Laboratory of Catalyst Supports Synthesis	**Head: Emmanuil A. Levitskii**
Laboratory for Catalyst Activity Testing	**Head: Dr. Nikolai N. Bobrov**

Group of Exothermic Reactions	**Head: Dr. Nikolai N. Kundo**
Laboratory of High-Temperature Catalytic Processes	**Head: Dr. Vyacheslav N. Gavrilin**
Laboratory of Unsteady-State Processes	**Head: Prof. Yurii Sh. Matros**
Laboratory of Catalytic Heat Generators	**Head: Dr. Zinfer R. Ismagilov**
Laboratory of Reactors for Catalytic Heat Generators	**Head: Dr. Alexandr D. Simonov**
Laboratory of Catalytic Conversion of Carbon Oxide	**Head: Prof. Tamara M. Yurieva**
Laboratory of Oxygen-Containing Organic Substances	**Head: Dr. Gennadii I. Panov**

DEPARTMENT OF HOMOGENEOUS AND COORDINATION CATALYSIS

Head: Prof. Yurii I. Yermakov (up to 1986)

Laboratory of Polymerization	**Head: Prof. Vladimir A. Zakharov**
Laboratory of Metal Organic Catalysts	**Head: Prof. Vladimir A. Likholobov**
Laboratory of Catalysis by Anchored Metal Complexes	**Head: Prof. Yurii I. Yermakov (up to 1986)**
Laboratory of Catalysis by Complex Metal Compounds	**Head: Prof. Klavdii I. Matveev**
Group of Organic Synthesis	**Head: Elena K. Mamaeva**

DEPARTMENT OF PHYSICOCHEMICAL METHODS FOR CATALYSTS INVESTIGATION

Head: Prof. Kirill I. Zamaraev

Laboratory of Investigation of Mechanisms of Catalytic Reactions	**Head: Prof. Kirill I. Zamaraev**
Laboratory of Spectral Methods	**Head: Dr. Eduard N. Yurchenko**
Laboratory of Quantum-Chemistry	**Head: Prof. Georgii M. Zhidomirov**
Laboratory of Adsorption	**Head: Prof. Anatolii P. Karnaukhov**
Laboratory of Structural Methods	**Head: Dr. Lyudmila M. Plyasova**
Laboratory of Analytical Chemistry	**Head: Dr. Vladislav V. Malakhov**
Laboratory of Catalytic Methods of Solar Energy Conversion	**Head: Prof. Valentin N. Parmon**
Laboratory of Mathematical Methods in Catalysis	**Head: Dr. Albert V. Fedotov**
Center of General Use	**Head: Dr. Vladimir N. Sidel’nikov**
Group of Heterophase Photocatalysis	**Head: Dr. Alexandr E. Cherkashin**
Laboratory of Automation	**Head: Dr. Yurii A. Alabuzhev**

DEPARTMENT OF KINETICS AND MATHEMATICAL MODELLING

Head: Dr. Alexey A. Ivanov

Laboratory of Multiphase Processes Modelling	**Head: Prof. Valerii A. Kirillov**
Laboratory of Processes Modelling in Fluidized Bed	**Head: Dr. Valerii S. Sheplev**
Laboratory of Kinetics	**Head: Dr. Alexey A. Ivanov**

DEPARTMENT OF CATALYTIC PROCESSES FOR PETROLEUM REFINING (in Omsk)

Head: Dr. Valerii K. Duplyakin

Laboratory of Catalytic Hydrocarbon Conversion	**Head: Dr. Valerii K. Duplyakin**
Laboratory of Catalytic Methods for Atmosphere Protection	**Head: Dr. Pavel G. Tsyrul'nikov**

DEPARTMENT OF INDUSTRIAL CATALYSTS

Head: Prof. Roman A. Buyanov

Group of Coordination on Application of the Achievements of Science to Production	**Head: Dr. Galina V. Glazneva**
Laboratory of Organization of Application of Scientific-Technical Developments	**Head: Dr. Vladimir A. Surikov**
Group of Attestation and Examination of Industrial Catalysts	**Head: Valerii P. Sokolov**

Pilot-Chemical Unit

Mechanical Shop

Electromechanical Unit

Glass-Blowing Shop

Metrological Shop

Preparatory Sub-Unit

SCIENTIFIC-SUPPORTIVE UNITS

Designing Bureau

Computer Center

Patent Office

Safety and Health Administration

Library of Scientific Literature

Editorship of Journal "React. Kinet. & Catal. Letters"

Editorial-Publishing Department

Printing Service

Administration and Services

MAIN ADVANCES OF THE INSTITUTE

In the frame of the problem **"Scientific Bases for Prediction of Catalytic Action"**

1. **The nature of active component of Cu-containing catalysts for methanol production** (chromites, ferrites, aluminates, solid solutions of magnesium and zinc oxides) has been investigated. The dependence of catalyst activity on the stability and dispersity of surface Cu-containing oxide compounds under reaction conditions has been revealed.

2. **The mechanism of catalytic activation of diatomic molecules at the surface of heterogeneous redox catalysts** (metals, oxides, nitrides) has been studied. The activation of dioxygen and dinitrogen molecules has been shown to proceed through reversible dissociative adsorption. It allows to predict catalytic properties of different chemical compounds for the reactions of ammonia synthesis and complete oxidation.

3. Considerable success has been gained in studying the **mechanism of catalysis by metal complexes**. Novel catalysts of practical importance – heteropolycompounds - have been developed to be used for production of monomers for thermostable polymers, semiproducts for vitamin synthesis.

4. A new type of elementary processes – **tunnel electron transfer** between the particles on the surface of heterogeneous catalysts – has been detected.

5. The general theory of **low-soluble hydroxides crystallization by mechanism of "oriented growing"** have been developed. The regularities obtained are used in purposeful synthesis of a series of supports and catalysts.

6. A new type of catalytic processes – **catalytic pyrolysis of hydrocarbons** – has been observed.

7. The detailed studies of an **effect of reaction medium** on vanadium catalyst for sulfur dioxide oxidation have been fulfilled.

8. The work has been done on studying **the mechanism of coking** – the main reason of deactivations of industrial catalysts for hydrocarbon processing.

9. The **quantum-chemical researches** allowed to obtain new data upon studying phenomenon of homogeneous and heterogeneous catalysis. An original concept of all chemical transformations in the system hydrocarbon molecule – Brönsted acid center through transient state of carbocationic type has been developed.

In the frame of problem **"Scientific Bases for Catalysts Preparation"** the methods are developed for preparation of:

Catalysts:

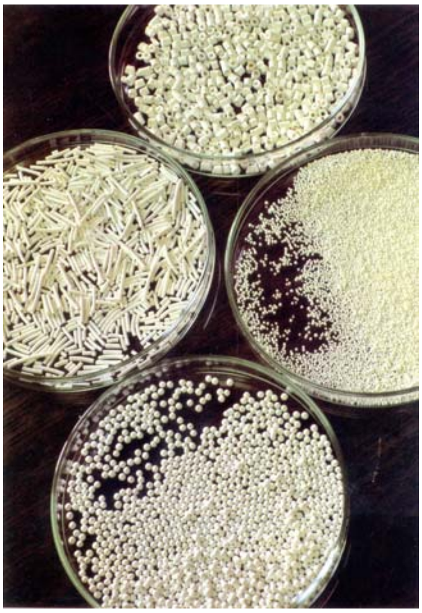
- **Mono- and bimetallic catalysts** for hydrocarbon conversion through anchored metal complexes;
- **Microspherical titanium trichloride** for ethylene polymerization**;**
- **Sn-Pt catalyst supported on Zn-Al spinel** for one-stage low paraffins dehydrogenation;
- **Nickel phosphate doped with gallium, antimony, tungsten oxides** (IC-25-2) for propane ammoxidation;
- **ICT-31-1** for methyl mercaptan synthesis from methanol and hydrogen disulfide and **ICT-32-1** for dimethyl sulfide conversion to methyl mercaptan;
- **Catalyst based on nickel, calcium and chromium phosphates** (IM-2206) to produce isoprene and butadiene;
- **Vanadium catalyst** IC-1-6 for sulfuric acid production**;**

- **Catalysts for hydrogenation** of nitrobenzotrifluoride to aminobenzotrifluoride**;**
- **Monolith catalysts** with low hydrodynamic resistance**;**
- **Zeolite-based catalysts** for production of liquid hydrocarbon fuel from natural gas and methanol;
- **Fe-Cr-K catalyst** for ethyl-benzene to styrene dehydrogenation**;**
- **V-Mg** and **Ti-Mg** catalysts for ethylene polymerization**;**
- **Photocatalysts** for hydrogen disulfide decomposition**;**

- **Supported metal catalyst** (Pd on various supports) with specific acid properties;
- **Al-Mn-O based thermally stable catalysts** for detoxification of sulfur-containing exhaust gases;
- **Ag-Mn catalysts** IC-3-11 and IC-3-12 for nitrose gases purification from oxygen;
- **Catalyst IC-11** for purification of exhaust gases from carbon oxide and organic impurities**.**

Supports:

- **Microspherical silica gel** for preparation of catalysts for gas-phase ethylene polymerization**;**
- **Microspherical alumina** for preparation of catalysts for ethylene oxichlorination;
- **Porous carbon material "Sibunit"** for preparation of Pd-based catalysts;
- **Carbon mineral sorbents** – highly stable supports with bifilic properties (SUMS-1).



SCIENTIFIC-SOCIAL LIFE OF THE INSTITUTE. KEY DATES

1980

March. Prof. Roman A. Buyanov became the Head of the Coordination Center of the member-countries of Soviet of Economic Mutual Assistance and Yugoslavia for the problem “Development of new industrial catalysts and improvement of the quality of catalysts applied in industry”.

October. The Institute received the International Award “Gold Mercury” for the productive development and international cooperation.

1981

July. The Center of General Use was organized. The main role of the Center became the organization of efficient operation of unique scientific devices to provide fundamental and applied investigations carried out by the Institutes. The Head of the Center became Vladimir N. Sidel’nikov. The center possessed NMR Spectrometer CXP-300, Mass-spectrometer MM 7070 HS, IR-Furier spectrometer IFS-113V, Digisorb-2500, Fluorimeter ORTEC-9200, Helium autopicnometer.

1982

November. An Agreement was signed between National Council on the Scientific Research and USSR Academy of Sciences on the scientific cooperation on the problem “Catalysis for Solving the Energy Problems ”. The Project Coordinators became the Institute of Energy Conversion and Storage, Messina and Institute of Catalysis, Novosibirsk.

1984

August. Academician Georgii K. Boreskov, initiator of the Institute and its permanent director since the date of its foundation, an eminent scientist with international recognition, has died.

October. Prof. Kirill I. Zamaraev became the Director of the Institute.

1985

December. The Institute of Catalysis became the leading institution of the Intersectorial Scientific-Technical Complex “CATALYST”, which combined efforts of 25 academician and applied-research Institutes. The main task of the ISTC “CATALYST” was to develop an efficient way of application of new catalysts and catalytic technologies to industry.

1986

June. Prof. Yurii I. Yermakov, deputy director, an outstanding scientists, has died.

July. Prof. Kirill I. Zamaraev became the Chief Director of the ISTC “CATALYST”**.**

1987

June 21-25. International G.K. Boreskov Memorial Conference “Modern Problems of Catalysis” was hold. The Conference was organized by the Institute of Catalysis under the auspices of the International Congress on Catalysis, USSR Academy of Sciences, SB USSR Academy of Sciences, Scientific Council on Catalysis of the USSR Academy of Sciences.

July. The intergovernmental Agreement was signed about scientific-technical cooperation between USSR and India. The long-term complex program was developed, which included the project “Catalysis”. Project Coordinators became the National Chemical Laboratory, Puna, and Institute of Catalysis, Novosibirsk.

August. Prof. Kirill I. Zamaraev was elected the President of the IUPAC Physical Chemistry Division.

1988

May. Grand meeting devoted to the 30th anniversary of the Institute of Catalysis.

Publications of BIC (Books and Monographs)

1979

“*Catalysts for the Processes of Sulfur Compounds Production and Conversion*”, Ed. **A.V. Mashkina**

“*Catalytic Synthesis of Organic Sulfur Compounds*”, Ed. **A.V. Mashkina**
“*Dynamic Regimes in Chemistry and Chemical Technology*”, Ed. **V.A. Chumachenko**

1980

V.N. Parmon, A.I. Kokorin, G.M. Zhidomirov, “*Stable Biradicals*”, “Nauka”, Moscow

Yu.I. Yermakov, V.A. Zakharov, B.N. Kuznetsov, “*Anchored Complexes on the Oxide Supports in Catalysis*”, “Nauka”, Novosibirsk

1981

G.K. Boreskov, “*Some Problems of Catalysis*”, “Znanie”, Moscow

D.G. Knorre, V.S. Muzykantov, “*Physical Chemistry*”, Textbook, “Vysshaya Shkola”, Moscow

E.N. Yurchenko, G.N. Kustova, S.S. Batsanov, “*Oscillating Spectra of Inorganic Compounds*”, “Nauka”, Novosibirsk

Yu.I. Yermakov, V.A. Zakharov, B.N. Kuznetsov, “*Catalysis by Supported Metal Complexes*”, Elsevier, Amsterdam, New York

V.A. Sazonov, T.L. Panarina, V.V. Popovskii, “*Commercial Catalysts for Gas Purification*”

Yu.N. Molin, K.M. Salikhov, K.I. Zamaraev, “*Spin Exchange: Principals and Applications in Chemistry and Biology*”, Springler, Berlin

"*Catalogue of Mass-Spectra*", Eds. **V.N. Sidel'nikov, L.V. Gur'yanova, V.A. Utkin, V.V. Malakhov,** "Nauka", Novosibirsk

1982

K.G. Ione, "*Polyfunctional Catalysis on Zeolites*", "Nauka", Novosibirsk

Yu.Sh. Matros, "*Unsteady Processes in Catalysis*", "Nauka", Novosibirsk

1983

R.A. Buyanov, "*Coking of the Catalysts*", "Nauka", Novosibirsk

V.A. Dzis'ko, "*Fundamentals of Catalysts Preparation*", "Nauka", Novosibirsk

G.S. Yablonskii, V.I. Bykov, A.N. Gorban', "*Kinetic Models of Catalytic Reactions*", "Nauka", Novosibirsk

G.S. Yablonskii, M.G. Kuz'min, S.D. Varfolomeev, "*Chemical and Biological Kinetics*", MSU, Moscow

1984

N.P. Keier, "*Studies of Catalysts Surface by Isotopic Methods*", "Nauka", Moscow

A.A. Davydov, "*IR-Spectroscopy in Studying the Chemistry of Oxide Surface*", "Nauka", Novosibirsk

A.I. Kokorin, V.N. Parmon, A.A. Shubin, *"Atlas of Anisotropic ESR Spectra of Nitroxide Biradicals",* "Nauka", Moscow

"*Mechanism of Catalysis. I. Nature of Catalytic Action, II. Methods of Catalytic Reactions Investigation*", Eds. **G.K. Boreskov, T.V. Andrushkevich**, "Nauka", Novosibirsk

"*Mathematical Modeling of Chemical Reactors*", Ed. **G.I. Marchuk**, "Nauka", Novosibirsk

1985

K.I. Zamaraev, R.F. Khairutdinov, V.P. Zhdanov, "*Electron Tunnelling in Chemistry. Long-Distance Chemical Reactions*", "Nauka", Novosibirsk

Yu.Sh. Matros, "*Unsteady State Processes in Catalytic Reactors*", Elsevier, Amsterdam

"*Photocatalytic Conversion of Solar Energy*", V. 1, 2, Ed**. K.I. Zamaraev,** "Nauka", Novosibirsk

"*Problems of Catalysts Deactivation. Nature of Specific Surface Activity*", Ed. **R.A. Buyanov**

"*Problems of Catalysts Deactivation. Structural Changes, Regeneration. Kinetics and Catalysts Modelling*", Ed. **R.M. Masagutov**

"*New Horizons in Catalysis*", Ed. **V.D. Sokolovskii**

1986

G.K. Boreskov, “*Heterogeneous Catalysis*”, “Nauka”, Moscow

E.N. Yurchenko, “*Methods of Molecular Spectroscopy in the Chemistry of Coordination Compounds and Catalysts*”, “Nauka”, Novosibirsk

A.N. Gorban’, V.I. Bykov, G.S. Yablonskii, “*Studies on Chemical Relaxation*”, “Nauka”, Novosibirsk

M.A. Fedotov, “*Nuclear Magnetic Resonance in the Solutions of Inorganic Compounds*”, “Nauka”, Novosibirsk

V.P. Zhdanov, “*The Rate of Chemical Relaxation*”, “Nauka”, Novosibirsk

1987

G.K. Boreskov, “*Catalysis. Theory and Practice*”, “Nauka”, Novosibirsk

Yu.Sh. Matros, “*Catalytic Processes under Unsteady Conditions*”, “Nauka, Novosibirsk

1988

G.K. Boreskov, “*Heterogeneous Catalysis*”, Ed. K.I. Zamaraev, “Nauka”, Moscow

V.P. Zhdanov, “*Elementary Physico-Chemical Processes on the Surface*”, “Nauka”, Novosibirsk

D.I. Kochubey, “*X-Ray Method to Study the Structure of Amorphous Materials: EXAFS-Spectroscopy”,* “Nauka”, Novosibirsk

S.P. Gabuda, R.N. Pletnev, M.A. Fedotov, “*Nuclear Magnetic Resonance in Inorganic Chemistry*”, “Nauka”, Moscow

CONFERENCE AND EXHIBITION ACTIVITY

Year	**Date**	**Event**
1979	13-15 February	All-Union Conference *"Unsteady Processes in Catalysis"* (more than 200 specialists in chemical technology and mathematical modeling)
	16-18 April	All-Union Conference *"Catalysis of Sulfur Compounds Reactions "* (110 specialists from academic and research institutes, enterprises)
1980	10-13 June	All-Union *Conference on Development of Productive Forces in Siberia*, Section "Chemical Industry"
	24 November- 5 December	All-Union School on Catalysts
1981	26-29 January	All-Union Seminar *"Isotope Methods in Studying Mechanisms of Catalytic Reactions"* (150 participants from Moscow, Leningrad, Alma-Ata, Sverdlovsk, Tomsk)
	12-18 March	Soviet-Czech Seminar *on Sorbents for Chromatography*
	8-11 June	III Ull-Union Conference *"Catalytic Purification of Waste Gases of Industrial Enterprises and Exhaust Gases of Motor Transport"* (more than 100 specialists from academic and applied institutions)
	18-25 June	*International School on Sulfur-Acid Catalysis* with participation of scientists from Poland. Czechoslovakia, and Yugoslavia
1982	21-25 April	III All-Russian Conference on *Mechanism of Catalytic Reactions* dated for the 75th Anniversary of G.K. Boreskov (more than 250 participants, among them scientists from Bulgaria, Hungary, Yugoslavia, Germany, France, Spain and Japan, 27 lectures, 55 short reports)
	14-16 December	2nd All-Union Conference "*Unsteady Processes in Catalysis*" (3 Sections: "Unsteady State of Catalyst", "Unsteady Processes in Chemical Reactors", "Optimization and Control of Unsteady Processes", about 150 participants)
1983	7-11 February	1st All-Union Conference "*Photocatalytic Conversion of Solar Energy*"
	1-7 July	VII All-Union Symposium "*Calorimetry in Adsorption and Catalysis*" (Irkutsk, Russia)
	12-14 December	All-Union Meeting "*Scientific Fundamentals of Catalysts Synthesis*"

1984	5-16 April	1st All-Union School on *EXAFS-Spectroscopy* (jointly with the Institute of Nuclear Physics)
	24-29 June	1st Soviet-Indian Seminar "*Catalysis and Advances in Chemical Technology*"
	8-12 October	1st Soviet-Italian Seminar *on Catalysis* (Messina, Italy)
1985	14-17 May	1st All-Union Meeting on the *Problems of Catalysts Deactivation* (jointly with the Ufa Institute of Petrochemical Production, Ufa, Bashkiria)
	24-27 September	All-Union Meeting "*Catalytic Heat Generators and Technological Processes on its Basis*"
	15-18 November	All-Union Seminar "*Heat Waves Propagation in Heterogeneous Medium*"
1986	15-19 July	5th International Symposium on *Relations between Homogeneous and Heterogeneous Catalysis* (37 plenary lectures and oral presentations, 267 poster presentations)
	21-24 October	3rd All-Union Conference "*Unsteady State Processes in Catalysis*" (13 plenary lectures, 190 poster presentations)
1987	13-16 April	2nd All-Union Conference "*Photocatalytic Conversion of Solar Energy*" (jointly with the Physics Institute of Leningrad State University, Leningrad)
	15-18 June	2nd Soviet-Italian Seminar "*Catalysis for Energy Problems Solving*"
	21-25 June	International Conference "*Modern Problems in Catalysis*" in Memory of G.K. Boreskov (more than 200 participants, among them 53 scientists from 17 foreign countries)
1988	6-13 July	International Exposition "Catalysis-88. Scientific Devices for Catalysts Production and Investigation" (63 firms from 11 countries)
	October	3rd Soviet-Indian Seminar "*Catalysis and Advances in Chemical Technology*" (jointly with the Institute of Inorganic and Physical Chemistry of Azerbaijan, Baku)

SCIENTIFIC DEPARTMENTS

DEPARTMENT OF PHYSICOCHEMICAL METHODS FOR CATALYSTS INVESTIGATION

HEAD OF THE DEPARTMENT PROF. DIMITRII I. KOCHUBEY

Laboratory of Structural Methods
Head: Dr. Sergey V. Tsybulya

Laboratory of Adsorption
Head: Prof. Valerii F. Yudanov

Laboratory of Analytical Chemistry
Head: Prof. Vladislav V. Malakhov

Laboratory of Spectral Methods
Head: Prof. Dimitrii I. Kochubey

Laboratory of Quantum Chemistry
Head: Prof. Georgii M. Zhidomirov

Surface Science Laboratory
Head: Prof. Valerii I. Bukhtiyarov

Laboratory of Investigation of the Mechanisms of Catalytic Reactions
Head: Prof. Eugenii P. Talsi

Group of the Mechanisms of Radical-Catalytic Reactions
Head: Dr. Vladimir A. Rogov

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

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

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

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

Study of the structural transformations in MnO_x/γ-Al_2O_3 system upon thermal activation has been an interest for the **Laboratory of Structural Methods** headed by Dr. S. Tsybulya**.**

MnO_x/γ-Al_2O_3 system is used as a catalyst for the processes of fuel combustion and VOC concentrated gas emission. Using *in situ* X-ray powder diffraction, high resolution electron microscopy and microanalysis the process of the solid phase transformations in this system at the calcination up to 1100°C has been studied. The structural mechanism of the thermal activation of manganese-alumina catalysts at the temperature range from 900 to 1000°C has been revealed in detail.

It was found that at these temperatures a solid phase reaction occurs along two different pathways: by diffusion of manganese ions into the structure of alumina (i) and diffusion of aluminum ions into manganese oxide (ii). Equilibrium biphase system composed of the cubic spinel $Mn_{1.5}Al_{1.5}O_4$ and α–Al_2O_3 that is in accordance with phase diagram is a final product of the solid phase interaction after prolonged (over 20 h) calcination of the manganese-alumina catalyst. Nanoheterogeneous state of the active component observed at the room temperature and up to 600°C is a result of the partial desintegration of the high temperature aluminum-manganese phase which is stable at the temperature of synthesis but metastable at the room temperature. Data obtained clearly show that manganese-alumina catalyst is a typical example of the nanostructural material.

Next methods were applied by the **Laboratory of Analytical Chemistry** headed by Prof. V. Malakhov to study composition of catalysts and reaction products:

- The method of differential dissolution (DD) was optimized based on the results of mathematical modeling and experimental studies of the DD process for the mixtures of phases with variable composition (with the constant and variable spatial distribution of components). The method is applied for detection stoichiometric and quantitative composition of such phases in complex heterogeneous catalysts (Al-Si systems, Fe-V-O, Cu-Zn-O, Li-Mg-Al-O and other).

- The upgraiding of two X-ray analyzers was accomplished (application of IBM, design of software and procedure for elemental analysis of the catalysts of different composition).
- Conditions were studied and optimized for preparation of capillary porous-layer columns with the film of sorbent from composite material on the base of the carbon. The columns are applied for improving the processes of chromatographic detection of composition of gas and liquid catalyzates.
- Methods are developed for preparation of high-speed multicapillary columns with polar and nonpolar liquid phases. The technology makes it possible to produce stright and U-shaped multicapillary columns 22-30 cm length with the efficiency up to 20000 theor. plates/m.

The following works have been carried out in the **Laboratory of Quantum Chemistry** headed by Prof. G. Zhidomirov during past year:

- Complexes of intermediate spin (S=3/2) iron ions emerging upon interaction of Fe^{2+} ions constituting FeZSM-5 zeolites with NO molecules are detected for the first time for oxide catalysts. This argues a possibility of stabilization of biologically similar spin states of iron ions in zeolite matrices.

- A new quasi-molecular concept of electrophilic oxygen O_{ep} was suggested. The concept allows basic experimental regularities of the epoxidation reaction to be described in unified terms.

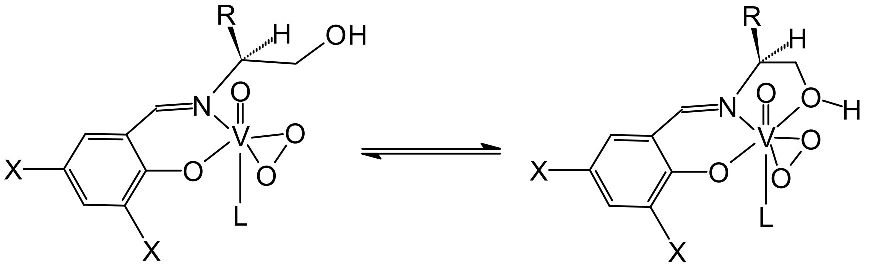
- An important theoretical prediction on the possibility of non-classical (“non-Bethe”) splitting of atomic terms in an electrostatic field of high symmetry was obtained.

Oxygen species realized in the course of ethylene epoxidation over silver have been studied at the **Surface Science Laboratory** headed by Prof. V. Bukhtiyarov in collaboration with Fritz-Haber-Institut der MPG (Berlin, Germany) using a number of physical methods sensitive to adsorbate electronic structure such as XPS, UPS, Auger and XANES spectroscopy. Namely, combined application of XANES and XPS in similar conditions using the same sample allowed us to assign spectral features to various oxygen species and make the conclusions about the nature of oxygen-silver bonding.

One of the species denoted as nucleophilic oxygen (E_b(O1s) = 528.4 eV) due to its activity in total oxidation only shows spectroscopic characteristics close to those of bulk Ag_2O. This allows us to describe this species as atomically adsorbed oxygen in the structure of surface silver (I) oxide. Considerable extent of the covalence in bonding of this oxide-like oxygen with silver surface due to hybridization of O2p levels with Ag4d and Ag5sp orbitals should be also emphasized.

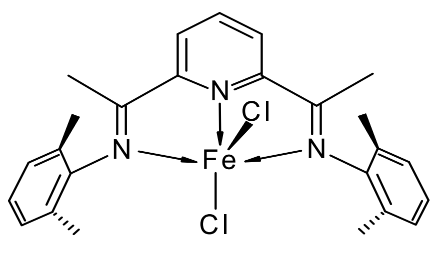
In-situ monitoring of O *K*-edge XAS spectrum of the pre-treated silver surface revealed a broad signal at 10-20 eV above the threshold. The comparison of the X-ray absorption spectra with O1s and valence band photoemission data allowed us to attribute this XAS signal to “electrophilic” oxygen (E_b(O1s) = 530.4 eV) which is known to be active in ethylene epoxidation. The complete absence of XAS features in the photon energy range typical for π* and σ* transitions of molecular oxygen (530 – 535 eV) indicates both the atomic origin of the electrophilic oxygen and the absence of molecular species on the catalyst surface under the present reaction conditions. Contrary to the nucleophilic oxygen, the electrophilic one does not exhibit hybridization of O2p levels with Ag4d, only Ag5sp orbitals participate in oxygen-silver bonding in this case. Photoemission data indicates higher degree of oxygen-silver bond covalence. The lower atomic charge on this O_{ads} explains the preference of its interaction with electron density of double C=C bond of ethylene with the formation of ethylene oxide. Possible models of adsorption centers for these oxygen species are discussed.

Catalytic system $[VO(Oi\text{-}Pr)_3]$/Chiral Shiff base/H_2O_2 of practical importance for enantioselective oxidation of sulfides was under studying at the **Laboratory of Investigations of Mechanisms of Catalytic Reactions** headed by Prof. E. Talsi using ^{51}V and ^{13}C NMR spectroscopy. Vanadium peroxocomplexes formed in the system were first characterized. Two types of the peroxocomplexes differing in the manner of coordination of the Shiff base to vanadium were shown to predominate in the system under study. The detected peroxocomplexes were found to be active species for enantioselective oxidation of sulfides (jointly with the Group of Catalytic Synthesis of Biologically Active Compounds).



A B

The structure of iron complexes formed during activation of ethylene polymerization catalysts based on bis(imin)pyridine complexes of iron by various co-catalysts ($AlMe_3$, MAO, $AlMe_3/B(C_6F_5)_3$, $AlMe_3/CPh_3B(C_6F_5)_4$) was first determined using ^1H and ^2H NMR spectroscopy. Neutral but, unlike the case of metallocenes, not cationic species were established to behave as active intermediates of polymerization (jointly with the Laboratory of Catalytic Polymerization).



The following works have been carried out by the **Group of Mechanisms of Radical-Catalytic Reactions** headed by Dr. V. Rogov:

- An installation for catalyst characterization using methods of temperature programmed reduction and temperature programmed reaction was adjusted and started-up. Activity of samples of exfoliated molybdenum sulfide supported in different materials was studied.

- A phenomenological scheme of formation of free radicals desorbed from the surface of Pt/SiO_2 and Pt/Al_2O_3 catalysts was developed. Experimental dependencies of the yields of methoxyl and methylperoxide radicals on the composition of the reaction mixture were explained in terms of the proposed model. Basic points of the model were supported by IR studies of *in situ* formed intermediates.

- Experiments on the choice of a standard source of alkyl and peroxide radicals to improve the technique for their direct mass-spectroscopic registration were carried out. It was discovered for the first time that the reaction of catalytic oxidation of propane proceeded in the autooscillation mode. The nature of the oscillations was shown to depend on pressure, reaction temperature and composition of the reaction mixture. The procedure for temperature determination of a metal catalyst based on the electric resistance was used to show that the oscillations of the reactant concentrations during the reaction were accompanied by periodical variations in the catalyst temperature while temperature of the gas phase remained constant.

The mechanism of the effect of structural transformations in adsorption layers on the adsorption rate and heat in the course of oxygen chemisorption on the surface (100) of metals was established by the **Group of Scanning Microscopy** headed by Dr. A. Salanov.

The **Laboratory of Texture Studies** headed by Prof. V. Fenelonov is traditionally engaged in works at two levels. First of them is certification of textural characteristics of catalysts, adsorbents and supports using standard techniques and Micromeritics instruments (nitrogen adsorption and mercury porosimetry).

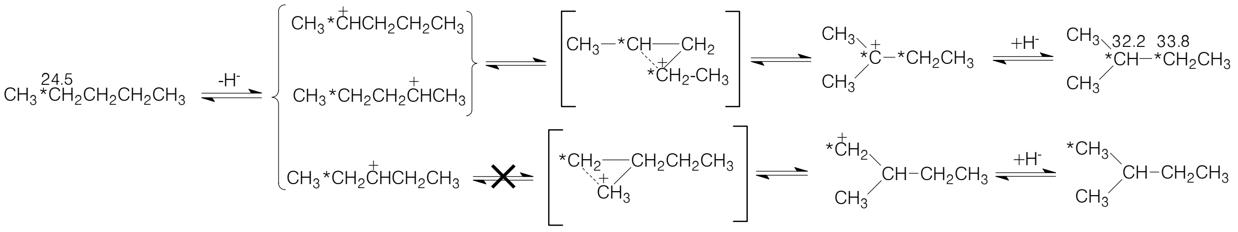
The second level is investigations of mechanisms of formation and evolution of porous textures or texture-dependent properties of porous solids. Poorly known systems and mechanisms are chosen for the studies using non-traditional and modified techniques. Among the latest problems under investigation are:

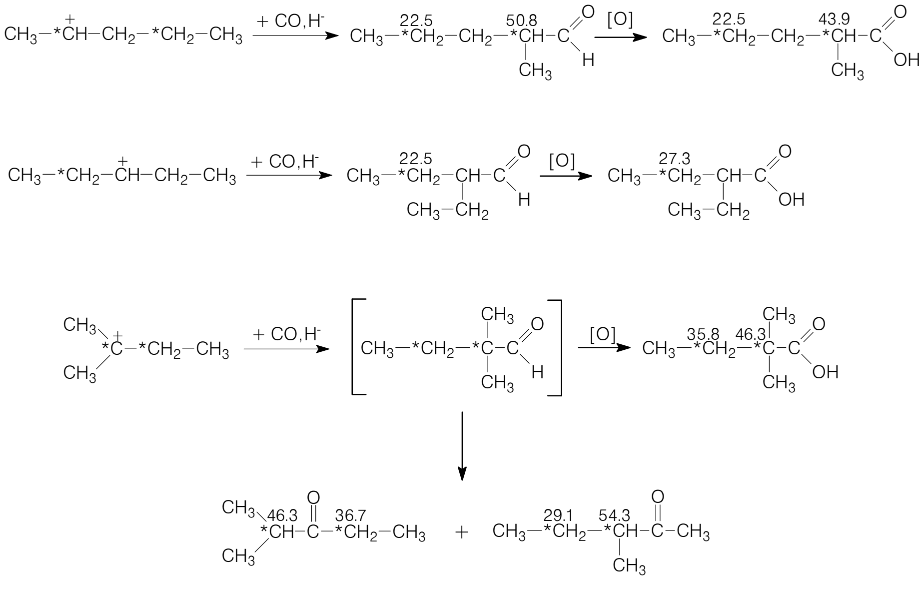
Mechanisms of texture formation in self-assembling systems such as mesoporous mesophases MCM-41, MCM-48, SBA-15 (in cooperation with the Group of Petrochemical Synthesis) and pillared layer systems (in cooperation with the Laboratory of Catalysts for Deep Oxidation). Combined XRD/N_2 adsorption method and the other are used to describe the textural characteristics.

Mechanisms of formation and properties of porous carbon materials. This is the filed under study for about a decade (monograph “Porous Carbon” by V. Fenelonov was published in 1995). The problems under current study are: a) storage of hydrogen and methane in carbon adsorbents, and b) synthesis of new carbon materials by carbonization in the porous space of MCM-41 and SBA-15 mesophases. Among the other problems under study are development of methods for separated measuring the surface of multicomponent systems including carbon/mineral sorbents and coke distribution in coked catalysts, as well as new approaches to the theory and practice of topochemical reactions accompanied by volume changes.

Among the pioneering results of the **Group of NMR Spectroscopy for Catalytic Hydrocarbon Conversion** headed by Dr. A. Stepanov are:

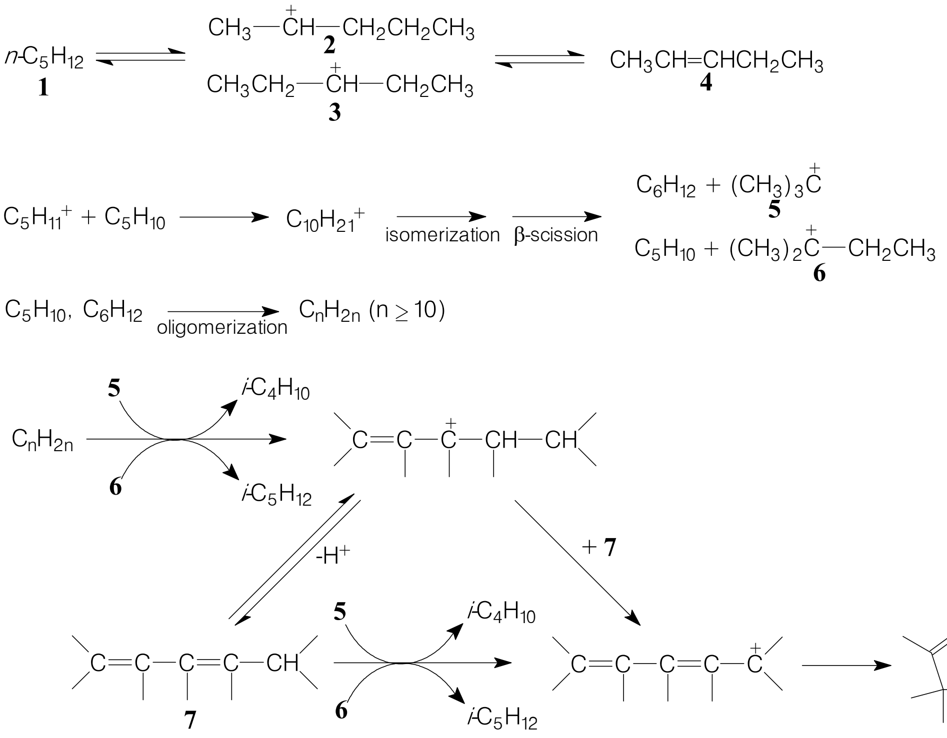
Carbonylation of *n*-pentane upon interaction with carbon dioxide over sulfated zirconia was established using *in situ* high resolution solid state ^{13}C NMR and *ex situ* liquid ^{13}C NMR techniques. Formation of a mixture of aldehydes, ketones and C_6-carbonylic acids was observed at 70°C in the absence of water but only C_6-carbonylic acids in the presence of water:





The direct spectroscopic evidence of the monomolecular mechanism of *n*-pentane isomerization over sulfated zirconia was obtained for the first time based on analysis of the observed specific distribution of the selective carbon label in the formed molecules of *iso*-pentane and carbonylation products.

In the absence of CO, transformation of pentane over SZ goes by two parallel routes: isomerization and the so-called “conjunct polymerization” according to the Scheme below. Both routes lead to formation of *iso*-pentane. The reaction of "conjunct polymerization" also produces products of pentane "disproportionation" (butanes and hexanes), as well as stable cyclopentenyl cations which cause the catalyst deactivation.



The **Group of Low-Temperature Catalysis by Metals** headed by Dr. V. Gorodetskii was concerned with:

Disappearance potential spectroscopy (DAPS) technique was used for systematic studies of electron properties of the Pt(100) surface during adsorption of H_2, O_2, NO and in the course of reactions H_2+O_{ads} and $NO+H_{ads}$. Satellite peaks assigned to conjugate electron exciting of valent electrons of adsorbed H, O, NO states were discovered. Intermediate $NH_{2,ads}$ species were shown to form in the course of $NO+H_{ads}$ interaction.

Reaction NO+CO proceeding on surfaces of Pt(100)-hex and Pt(100)-1×1 was studied in detail. As established before, successive filling of the Pt(100)-hex surface by NO and CO results in generation of surface islands of the 1×1 phase saturated with a mixture NO_{ads} and CO_{ads} molecules. A reaction between the adsorbed species is shown to occur in the mixed islands on heating and, independently of filling coefficients Θ_{NO} and Θ_{CO}, to look like a surface explosion. The starting temperature of the reaction is practically independent of the adsorbate concentrations ($T_{sur}\approx 390$ K) that is characteristic of TPR proceeding in locally unsaturated mixed adsorption layers. Different reaction mode is observed on the 1×1 surface with the statistical distribution of NO_{ads} and CO_{ads} characteristic of it. First of all, an extremely high catalytic activity with respect to reaction NO+CO is demonstrated for this surface: quantitative titration of NO_{ads} with carbon monoxide and back is observed at the temperature as low as 300 K. As to mixed NO_{ads} and CO_{ads} layers prepared on the 1×1 surface at T>250 K, the reaction occurs on heating and is fixed as narrow peaks of products which look like peaks of surface explosion at the *hex* surface. However, the position and width of the peak depend on a total of concentrations of the adsorbed species, $\Theta_{NO}+\Theta_{CO}$. This dependence is determined by contribution of unoccupied adsorption sites to the key reaction stage, *i.e.* dissociation of NO_{ads}: the lower $\Theta_{NO}+\Theta_{CO}$, the lower is the reaction temperature and the wider peak. In the limit of the saturated coverage ($\Theta_{NO}+\Theta_{CO} \approx 0.5$ ML), the reaction temperature and peak widths reach the values obtained for the surface explosion at the *hex* surface.

Modifying influence of Pd on the nature of active Ti^{3+}-□ sites in the system of Pd/Ti^{3+}-□/TiO_2 was studied using the spillover effect: metal $\rightleftharpoons$ support. Oxygen is shown to be adsorbed at 100 K as two molecular γ- and α-species (desorption temperatures T_{des}~140 and 240 K, respectively) on a thin oxide layer TiO_x (~300 Å) containing surface defects Ti^{3+}-□ (where □ is an oxygen vacancy) in a high concentration. Exposure to light at the energy range of $2.8<h\nu<3.4$, that is close to the TiO_2 band gap width, leads to photodesorption of the α-species resulting from the reaction between a light-generated hole and α-$O_2^{-\delta}{}_{ads}$. Supporting of Pd in the form of ca. 20Å particles gives rise to the following phenomena: (i) stabilization of surface Ti^{3+} defects (SMSI effect); (ii) an increase in the stability of α-oxygen up to T_{des}~500 K. α-O_{2ads} species on TiO_x appear inactive with respect to the reaction with H_2 that is accounted for by the absence of sites for dissociation of hydrogen molecules. The reaction of α-oxygen with H_2 over the Pd/Ti^{3+}-□/TiO_2 system at 150 K is caused by the spillover effect, *viz.* diffusion for H_{ads} atoms from Pd particles to the TiO_x surface. The following series of activities to stationary oxidation of H_2 was established: Ti^{3+}-□ (TiO_2) << Pd ≈ Pd/Ti^{3+}-□/TiO_2.

DEPARTMENT OF NONTRADITIONAL CATALYTIC TECHNOLOGIES

HEAD OF THE DEPARTMENT ACAD. VALENTIN N. PARMON

Laboratory of Catalytic Methods of Solar Energy Conversion

Head: Acad. Valentin N. Parmon

Laboratory of Energy Transforming Materials

Head: Dr. Yurii I. Aristov

Group of Aerogel Materials

Head: Dr. Aleksandr F. Danilyuk

Group of Photocatalysis on Semiconductors

Head: Prof. Eugenii N. Savinov

Laboratory of Catalytic Processes for Desulfurization

Head: Prof. Nikolai N. Kundo

Group for Stereoselective Catalysis

Head: Dr. Oxana A. Kholdeeva

Group of Aerosol Catalysis

Head: Dr. Valerii N. Snytnikov

Group of Biocatalysis

Head: Dr. Galina A. Kovalenko

Energy-Chemical Engineering Group

Head: Prof. Vladimir I. Anikeev

The **Laboratory of Catalytic Methods of Solar Energy Conversion** headed by Acad. V. Parmon has been engaged in the following research projects:

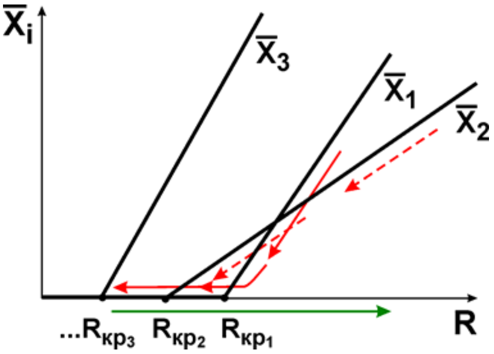
- The method of kinetic analysis of a homogeneous system comprising simultaneously several types of non-interacting molecules-autocatalysts X_i generated in the course of chemical transformations of the same substrate-“food” R is used to show that the phenomenon of unidirectional natural selection of the autocatalysts may emerge that provides, when mutations of the autocatalyst molecules can occur, fixing of the acquired properties. This conclusion on the potentiality of fixing the acquired properties in simple chemical systems with no constituent bearing the biological information, such as DNA, is of crucial importance to developing the realistic scenarios for the natural origin of life.

$$R + X_i \underset{k_{-i}}{\overset{k_i}{\rightleftarrows}} 2X_i$$

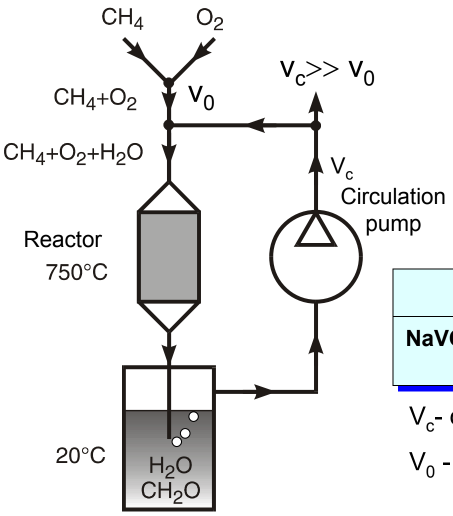
$$X_i \xrightarrow{k_{ti}} P$$

$$\bar{X}_i^{(1)} = \frac{k_i}{k_{-i}}\left(R - \frac{k_{ti}}{k_i}\right) \equiv \alpha_i\left(R - R_{кр_i}\right)$$

$$\bar{X}_i^{(2)} = 0$$



- The improved catalytic process for oxidation of methane by oxygen into formaldehyde using a flow circulating reactors and the procedure of water quenching of the reaction mixture at room temperature was shown to allow 100% selectivity to formaldehyde at temperatures of 650–750°C.



$$CH_4 + O_2 \rightarrow CH_2O + H_2O$$

Catalyst	S_{CH_2O}, %	Y_{CH_2O}, %
$NaVO_2SO_4$+$K_3VO_2S_2O_7/SiO_2$ (IC-1-4, IC-1-6)	100	60

V_c- circulation rate

V_0 - reaction mixture feed rate

- Thermal activation of aluminium hydroxide, $Al(OH)_3$, by heating it at the rate higher than 500°/s is the key stage of preparation of active alumina, which is an important semiproduct used for synthesis of basic types of catalyst supports. An experimental unit of a centrifugal reactor, a fundamentally new device for thermal activation of alumina, was designed in cooperation with the Design Technological Institute of Hydropulse Techniques (Novosibirsk) and assembled. Preliminary studies of the phase composition and physicochemical properties of prepared active alumina samples were carried out.

The following results were obtained by the **Laboratory of Energy Transforming Materials** headed by Dr. Yurii I. Aristov**:**

- The dynamics of carbon dioxide sorption by composite sorbents based on a potassium carbonate dispersed in different porous matrixes (silica gel, aluminas, vermiculate, Sibunit) has been studied at 400°C. A set of methods (X-ray diffraction, thermogravimetry, low-temperature nitrogen adsorption and TEM) were used to study the structural and chemical transformations in the composite sorbents based on alumina. For these sorbents the dynamic sorption capacity was shown to achieve 0.1 g/g. The optimal regeneration procedure is suggested. The sorbent operation under PSA mode is studied.
- New selective water sorbents based on the vermiculate or MCM-41 as host matrices and calcium chloride as a hygroscopic salt are synthesized. Water sorption isobars, isosters and isotherms have been measured and analysed. The isosteric sorption heat is measured to be 65-70 kJ/mole and 40-45 kJ/mole at low and high water uptakes. The formation of stable crystalline hydrates containing 1/3 and 1 molecule of water inside vermiculate pores has been shown. The application of $CaCl_2$/MCM sorbent in sorption refrigerating units is analyzed.
- An effecient coefficient of heat conductivity λ of the system "silica gel KSK + calcium chloride" has been measured by the "hot wire" method at T=293 K. It is found that the heat conductivity gradually increases with the raise of the water uptake *w*. The sharp increase in λ is observed when a continuous phase of aqueous salt solution is formed inside the silica pores. The results obtained are satisfactorily described by Luikov-Bjurstrom model.
- Analytical equations of Henry, Freundlich, Dubinin – Astakhov, Brunauer – Emmett – Teller and a new modification of the BET equation are used for thermodynamic description of water activity over wide temperature (260 – 600 K) and water mole fraction (0.3 – 0.8) ranges for concentrated aqueous solutions of electrolytes. The solutes considered are H_2SO_4, $CaCl_2$, LiBr, LiCl, LiI, $MgCl_2$ and NaOH in bulk state and $CaCl_2$, LiBr in dispersed state. The generalized Henry equation is found to allow a correct extrapolation of the bulk solution properties measured at low and moderate salt concentrations to the region of low water contents. The suggested modification of the BET equation as well as the Dubinin – Astakhov equation give a precise (with a relative error less than 1 %) description of literature data on the "humidity – concentration" dependence and can be used for the reliable prediction of this dependence in the region of intermediate conditions.
- Energy storage ability E is measured over T = 50-340°C for more than fifteen samples of selective water sorbents based on silica gels, aluminas, carbon Sibunit and aerogels as host

matrices and $CaCl_2$, LiBr, $MgCl_2$ as impregnated salts. The E-values up to 8.4 kJ/g and 4.0 kJ/g are found for forced and naturally saturated sorbents that are much higher than for common materials. These values make the sorbents promising for long-term energy storage. The temperature dependence of E gives an estimation of sensible and latent heat contributions as well as the specific heat of a dry sorbent. The relation between the energy storage ability and water content allows to obtain the heat of water desorption and can be used for brief estimation of energy storage ability for a variety of SWS composites.

- The pilot production of composite sorbent SWS-1L (IC-11-2) based on silica gel as porous host matrix and calcium chloride as active substances is commercialized jointly with Omsk Division of Boreskov Institute of Catalysis.

The **Group of Aerogel Materials** headed by Dr. A. Danilyuk continued studying the effect of sol-gel preparation conditions on the alcogel structure formation and its evolution upon aging. Based on the results obtained, an improved method for aerogel synthesis was suggested. This method allows to prepare the aerogels with the light-scattering length more than 50 mm. High light scattering length is an important characteristic of aerogels used in Cherenkov counters.

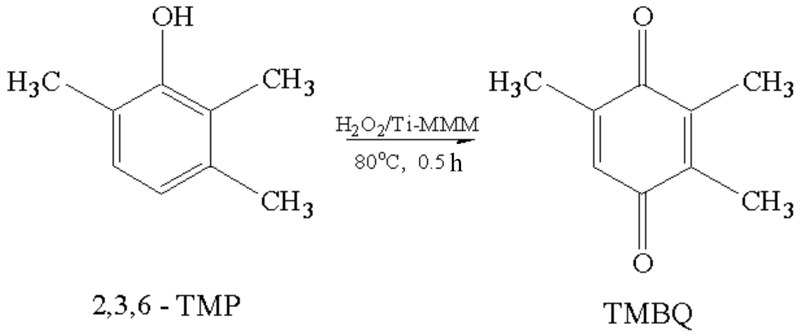
The mechanism of supramolecular crystallization of monodispersed spherical silica particles suspensions has been studied jointly with the Institute of Mineralogy and Petrography (Novosibirsk). The crystallization of the particle suspension in diethyl ether has been studied for the first time. It was found that the linear crystal growth rate depends on temperature. The linear law of the crystal growth is associated with diffusion of the structural units on the interface.

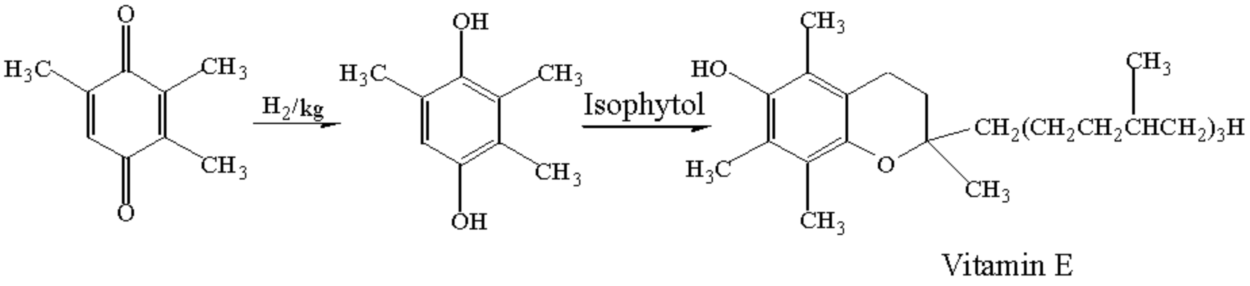
The research work of the **Laboratory of Catalytic Processes for Desulfurization** headed by Prof. N. Kundo was aimed at the following subjects:

- The reaction of gas-phase oxidation of hydrogen sulfide at temperatures below the dew point was shown to produce elemental sulfur through formation of polysulfides as intermediates. The reaction stages were suggested implying that elemental sulfur and SO_2 are formed by concurrent reactions from H_2S, elemental sulfur being formed from the polysulfide intermediates. A catalyst was developed for low-temperature oxidation of H_2S. It can be used to substitute for the currently employed imported catalyst AM for removal of oxygen trace, as well as for absorption of H_2S from waste gases of the Claus process.
- A method for synthesis of Al-Cu-Cr catalysts from tailings of galvanic industry was developed on the basis of the technology for preparation of catalyst ICT-12-8. The activity and strength of experimental samples of the catalysts are not lower than the corresponding parameters of ICT-12-8.

The **Group for Stereoselective Catalysis** headed by Dr. O. Kholdeeva studied the catalytic properties of mesoporous mesophase systems of silicate materials containing Ti(IV) and V(V) ions (Ti- and V-MMM) in oxidation of 2,3,6-trimethylphenol (TMP) and 2-methylnaphtalene

(MN) with hydrogen peroxide and *tert*-butylhydroperoxide. Oxidations with H_2O_2 over Ti-MMM, unlike the reactions over V-MMM, were established to be true heterogeneous processes, no titanium leaching occur from the solid matrix into the solution. The reaction conditions and catalyst composition were optimized for the TMP oxidation. The titanium content in the catalyst, TMP concentration, solvent nature and the reaction temperature were found to be the key factors affecting the process selectivity. Under the optimal conditions, the target product – trimethyl-*para*-benzoquinone (TMBQ) – could be obtained with the selectivity of 86% at 100% TPM conversion. The method for TMBQ preparation was first developed using a really heterogeneous catalyst. Physicochemical techniques (XRD, DRS-UV) were used to establish relationships between the composition of Ti-MMM catalysts, their structure perfection, the state of the active catalytic site and catalytic properties. The highest activity and selectivity were observed with Ti-MMM samples containing 1.5-2% of Ti, in which isolated state of the titanium and high structural ordering of the silicate matrix were provided. The use of concentrated hydrogen peroxide allowed the catalyst lifetime to be extended.





Solvent	AcOH, MeCN, MeOH
TMP conversion	100%
Selectivity	86%
Catalyst efficiency	17 (mol TMBQ/mol Ti × h)
Productivity	310 (g TMBQ/l/day)

Advantages

- Catalyst is separated by filtration and may be used repeatedly
- No admixtures of heavy metals in the product
- Ecologically sound and inexpensive oxidizer
- No Cl-containing reagents and solvents

$\Rightarrow$ High product purity

Experimental studies of resonance absorption in gas were carried out by the **Group of Aerosol Catalysis** headed by Dr. V. Snytnikov using a CO_2-laser of 100 Wt capacity designed and put into practice. Gaseous reactants were heated using the laser with the power density of the energy flux up to 200 Wt/cm^2 that was higher by more than an order of magnitude than the fluxes achieved in industrial chemical reactors. Pyrolysis of methane was detected. Thus, feasibility of studies of endothermic reactions, such as steam and carbon dioxide conversion of methane and others, under fundamentally different conditions of energy supply was demonstrated.

Experimental evidence was obtained that laser-induced fluorescence diagnosis based on a pulse excimer laser, as one of the most sensitive methods, can be used among main tools for studying microsecond chemical reactions for two-phase flows.

Development of the numerical code for simulation of the space chemical reactor of the protoplanetary disk was continued. The set of Liuville-Vlasov equations and the Poisson three-dimensional equation was supplemented with gas dynamic equations.

Comparative studies of adsorbents based on catalytic filamentous carbon (CFC-1 and CFC-2) are carried out by the **Group of Biocatalysis** headed by Dr. G. Kovalenko (jointly with the Laboratory of Catalytic Processes in Dynamic Bed)**.** The discovered feature distinguishing these materials from granulated carbon-based supports (SUMS, Sibunit) is their high efficiency in adsorption of biologically active substances (amino acids, proteins, bacterial cells). Comprehensive studies of adsorption properties of CFC led to the following conclusions:

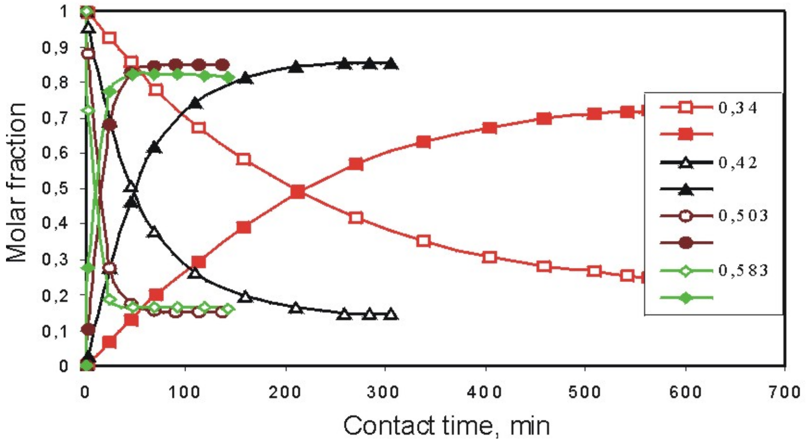
- The key factor determining adsorption of amino acids (L-tyrosine) and protein molecules (albumin, glucoamylase) on the surface of CFC-1 and CFC-2 is the area of accessible surface of the support, which depends on the porous structure: occurrence of size-fitting pores provides effective and strong adsorption along with maximal stabilization of the enzyme reactivity;
- The key factors determining adsorption of bacterial cells on the CFC surface are the area and roughness of the accessible surface of supports under study. The accessible surface area appropriate for adsorption of large objects such as a bacterial cell (1 to 6 μm size) was determined using three independent techniques including comparative and fractal methods. The surface roughness was controlled by varying the carbon yield (g of carbon per 1 g of support): as this parameter increased, the surface became more dense and smooth. Experimental and electron microscopic studies revealed that an increase in the surface

roughness resulted in an increase in the amount and strength of adsorption of bacterial cells on CFC.

Adsorption of amylolytic enzymes on inorganic differently shaped aluminosilicate granules with the surface covered by catalytic filamentous carbon was studied in order to develop a heterogeneous biocatalyst for the process of starch hydrolysis to glucose (jointly with the Group of Dynamics of Surface Transformations). Adsorptive immobilization of glucoamylase on these supports was shown to result in dozens-fold increase in the stability of this enzyme. For example, the inactivation halftime ($t_{1/2}$) at 65°C was 0.5 h for the soluble enzyme but 9.5 h for immobilized glucoamylase.

Studies of biocatalytic properties of propane-assimilating *Rhodococcus rubber* bacteria (with the culture donated by the unique regional collection of alkanotrophic microorganisms of the Ural Branch of the RAS, Perm) showed that these microorganisms revealed intracellular *monooxygenase* enzymatic activity. Conditions (composition of the medium, temperature regime, growth time) were chosen for cultivation of the bacteria in order to provide the maximal activity of the Rhodococcus cell suspension. The chosen growth conditions allowed high-selective bioepoxidation of propylene to be achieved at the rate of 10 nmol/min/mg of dry cells that was some times as high as the best literature data.

Based on the studies of the 2-propanol dehydration reaction in supercritical water (SCW) the **Energy-Chemical Engineering Group** headed by Prof. V. Anikeev showed that, first, the reaction mechanism differs considerably from that in the presence of a homogeneous acid catalyst and, second, the reaction rate and equilibrium constant depend on the SCW density. Basic mechanism of 2-propanol dehydration of in supercritical water was suggested based on experimental data on the reactions of hydration and hydrogenation of the main products of the target reaction. It was shown that regular local density could be formed in the bulk of the supercritical fluid due to dissipation of the mechanical energy.



Dehydration of 2-propanol in SCW at 393°C. Molar fraction of 2-propanol (void symbols) and propylene (solid symbols) *versus* contact time with SCW by different densities (0.34, 0.42, 0.503 and 0.583 g/ml).

A thermodynamic approach was developed for computing simultaneous chemical and phase equilibrium in multiphase mixtures. The proposed method was implemented with the reaction of benzene hydrogenation as an example; the reaction was achieved using a flow (with respect to liquid and gas) ideal mixing reactor under conditions of the phase equilibrium at the outlet. The task of defining stationary states was accomplished. The reason for the multiplicity of stationary states and for the presence of the range of unstable solutions was shown to be the non-linear dependence of the reaction rate on reactant concentrations in the liquid phase, deviation of the properties of the formed liquid phases from the properties of the ideal state affecting the process of hydrogen dissolution in the liquid reaction medium, the occurrence of the azeotropic point in the binary mixture of benzene and cyclohexane. The influence of non-ideality of the reaction mixture on the equilibrium composition of ammonia and methanol synthesis reactions was illustrated. Computed and experimental data were compared.

DEPARTMENT OF HETEROGENEOUS CATALYSIS

HEAD OF THE DEPARTMENT PROF. VLADIMIR A. SOBYANIN

Laboratory of Catalytic Processes in Fuel Cells
Head: Prof. Vladimir A. Sobyanin

Laboratory of Catalysts Preparation
Head: Prof. Oleg P. Krivoruchko

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

Laboratory of Heterogeneous Selective Oxidation
Head: Prof. Tamara V. Andrushkevich

Laboratory of Dehydrogenation
Head: Prof. Roman A. Buyanov

Laboratory of Oxidative Catalysis over Zeolites
Head: Prof. Gennadii I. Panov

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

Laboratory of Catalytic Heat Generators
Head: Prof. Zinfer R. Ismagilov

Group of Direct Catalytic Hydrogen Sulfide Oxidation
Head: Dr. Mikhail A. Kerzhentsev

Laboratory of Catalytic Conversion of Carbon Oxides
Head: Prof. Tamara M. Yurieva

Group of Reactions of Oxidation on Metals
Head: Prof. Aleksandr V. Khasin

Group of Catalytic Synthesis of Oxygen-Containing Compounds
Head: Dr. Galina G. Volkova

Group of Dynamics of Surface Transformations
Head: Dr. Andrei V. Simakov

Studies of the electrocatalytic methane-to-syngas oxidation over Pt- and Ni-ceramic electrodes supported on solid oxygen-conducting electrolyte has been completed in the **Laboratory of Catalytic Processes in Fuel Cells** headed by Prof. V. Sobyanin. It has been shown that Pt-ceramic electrode at electrocatalytic oxidation of methane in a dilute absence provides simultaneous generation of electricity and syngas production with high output (up to 92%). Under these conditions Pt-ceramic electrode is stable and coking resistant.

Systematic investigations of the reaction of dimethylether (DME) steam reforming to hydrogen-rich gas mixture were fulfilled. It has been shown for the first time that mechanic mixture of catalysts for DME hydration to methanol and for steam conversion of methanol provides an efficient steam reforming of DME to hydrogen-rich gas. The catalysts allowing to obtain hydrogen-rich gas with H_2 concentration ~75 vol.% at 250-280^{o}C have been proposed.

The studies of the **Laboratory for Catalyst Preparation** headed by Prof. O. Krivoruchko were focused on:

- The influence of the nature of elements of II Group and surfactants (polyvinyl alcohol and polyethylene oxide) on the formation of phase composition, dispersion and porous structure of zirconium-containing systems M-Zr-O, where M was Ca, Sr, Ba has been revealed. The distinguishing feature of the structures formed in the presence of the surfactants was shown to be their ordering and double lattice constant of the solid solution, the constant being increased in a regular manner in the series of Ca $\longrightarrow$ Sr $\longrightarrow$ Ba in accordance with their ion radii.

- A method was developed for preparation of granulated V-Ti-Mo catalyst with optimal structural and mechanical properties for synthesis of nicotinic acid by gas-phase direct oxidation of β-picoline. A higher yield (80-82%) of nicotinic acid and a higher productivity were observed with the granulated V-Ti-Mo catalyst in comparison with the binary V-Ti catalyst.
- Thin-wall graphite nanotubes were first synthesized by catalytic transformation of a three-dimensional matrix of amorphous carbon over an iron-containing catalyst in flowing nitrogen at 600-750°C.
- ^{11}B, ^{23}Na, ^{27}Al, ^{29}Si NMR, IR and TEM spectroscopies, BET, TPD techniques were used for studying regularities of genesis, physicochemical nature and structure of silica supports produced by leaching B-Si and Na-Si fiberglass materials.

Regularities of selective dehydrogenation of diethyldisulfide into ethanethiol in the presence of transition metals supported on various carries were investigated by the **Group of Catalytic Transformations of Sulfur-Containing Compounds** headed by Prof. A. Mashkina. Factors affecting the reaction pathway were established. Feasibility of catalytic hydrogenation of some spatially hindered phenols into alkylarylthiols (prospective as stabilizers in polymerization processes) was demonstrated.

The **Laboratory of Heterogeneous Selective Oxidation** headed by Prof. T. Andrushkevich proceeded in studying mechanisms of reactions of partial oxidation over heterogeneous catalysts.

Oxide binary V_2O_5/Me_xO_y (Me_xO_y = MgO, TiO_2, Sb_2O_3, MoO_3, P_2O_5) and MoO_3/P_2O_5 systems, heteropolyacids and salts were studied in the oxidative ethane conversion. V-Mo-O system with high molybdenum content ($10V_2O_5$ - $90MoO_3$, % mass) has been shown to be the most efficient. The yield of ethylene amounts 30% at $T=400^oC$.

The relaxation of multicomponent catalysts based on iron antimonate was studied in the reaction of propylene ammoxidation. At constant composition of reaction mixture the stationary catalysts state is determined by the degree of conversion: the higher is the degree of conversion, the higher is the degree of catalyst reduction. The time of catalyst relaxation from stationary state, corresponding to high conversion degree, to the state corresponding to low conversion is long, about tens seconds.

The surface complexes of 3-methylpyridine (3-MP) over vanadia-titania catalysts for nicotinic acid production have been detected using Fourrier IR spectroscopy *in situ* in temperature range 100-300^{o}C. Two molecularly bond with catalyst complexes were identified: 3-methylpyridinii ion, formed upon 3-MP interaction with hydroxyl groups, and 3-MP coordinatively bond with Lewis acid centers.

In this case disturbance of the C-H bond in methyl groups also is observed. As temperature is elevated to 150°C, the methyl is oxidized into carbonyl group that is argued by antibate variations in the a.b. of deformation $\delta_{C\text{-}H}$ oscillations in the CH_3-group and valent $\nu_{C=O}$ oscillations. The intensity of a.b. of carbonyl group decreases at the temperature range of 200-280°C, while absorption bands of carboxyl group, which are characteristic of the spectrum of nicotinic acid, appear. Only slight changes in the position of a.b. of aromatic ring are observed at the temperature range under study (50-280°C) during all the above-described transformations. Similar transformations of the carbonyl to carboxyl groups are observed at the same temperature range upon interaction of pyridine-3-carbaldehyde with the vanadium-titanium catalyst.

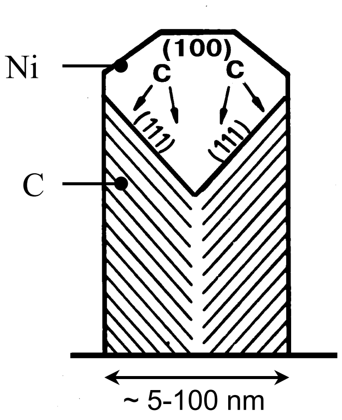
The **Laboratory of Dehydrogenation** headed by Prof. R. Buyanov was engaged in research in the areas:

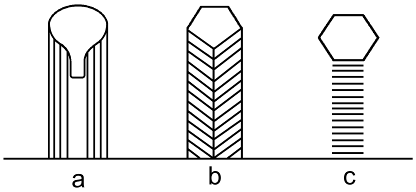
- The process of filamentous carbon formation from carbon atoms, generated upon catalytic decomposition of hydrocarbons on the iron group metals according to carbide cycle mechanism, is studied in detail. The growth models of some morphological modifications of important nanomaterial – nanofilaments with coaxial-cylindrical, coaxial-conical and starched disposition of carbon basal layers are developed.

Carbide cycle of carbon atoms formation from butadiene :

$$Fe + C_4H_6 \xrightarrow{-H_2} [Fe\text{–}C] \rightarrow Fe + C$$

Model of filamentous carbon growth over nickel nanoparticle

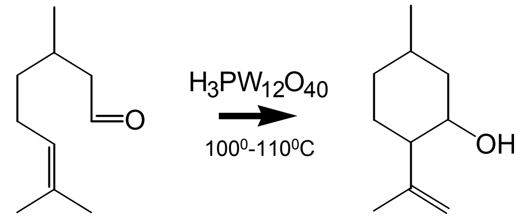




Longitudinal profile of main types of carbon nanofilaments and spatial arrangement of basal graphite planes:

a) Concentric cylinders, parallel to the nanofilament axis
b) coaxiall cone-shaped planes;
c) plane graphite layers, perpendicular to nanofilament axis

- New efficient catalysts (P-W-HPA) for citronellaldehyde cyclization to isopulegols for synthesis of menthol – valuable fragrant and medicinal product - are developed. The advantages of these catalysts are: 2-4 fold shortening of the time of synthesis; no corrosion medium and wastes; easy catalysts separation from reaction medium. A novel method for L-isopulegol synthesis to produce L-menthol is suggested. It is based on the isomerization of other isopulegols over heteropoly catalyst.



citronellal

L- and D-isopulegols

Separation of L - isopulegol from the mixture of isopulegol isomers after citronellal cyclization

⇓

Isomerization of other isomers

⇓

Separation of L - isopulegol from the mixture of isomers

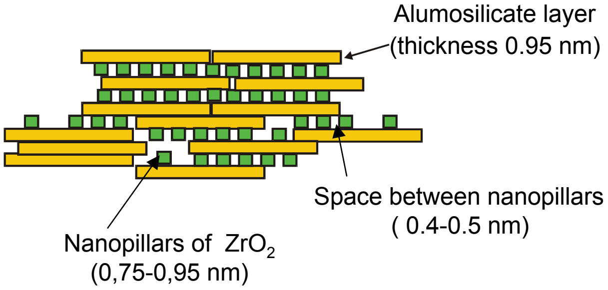
Advantages

- Complete use of feedstock
- Low temperatures
- Shortening of the time of synthesis

- A laboratory evaluation unit for neutralization of high-toxic and ecologically harmful organochlorine wastes was designed and tested. The process is based on catalytic pyrolysis or high-temperature hydrodechlorination. Feasibility of two modes of the utilization process at the waste conversion close to 100% was demonstrated.

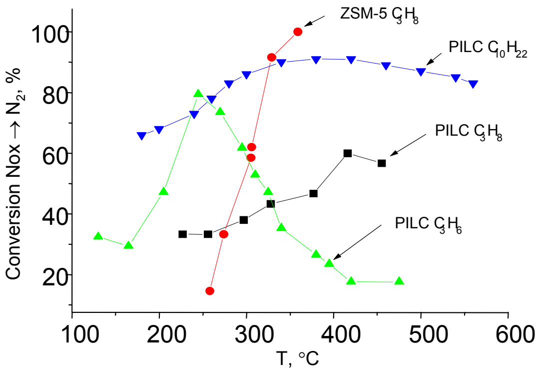
Pt-promoted cation- and anion-modificated fluorite-like solid solutions based on cerium dioxide, which possess high mobility of lattice oxygen, were studied in the **Laboratory of Catalysts for Deep Oxidation** headed by Prof. V. Sadykov. The possibility to obtain syngas from methane by its non-stationary selective oxidation to CO and H_2 by oxygen of catalyst crystal lattice with subsequent aqueous reoxidation has been shown. The developed systems are stable to coking and sintering.

Pillared clays structure



Typical temperature dependencies of nitrogen oxides reduction by hydrocarbon over pillared clays in reaction

$$CH_x+O_2+NO_x \Rightarrow N_2+H_2O+CO_2$$



Thermally stable (up to 700°C) microporous materials - pillared montmorillonite clays intercalated with partially stabilized zirconium dioxide nanoparticles were successfully synthesized. An efficient catalyst for selective nitrogen oxides reduction by heavy hydrocarbons (decane) in oxygen excess has been developed.

The **Laboratory of Catalytic Heat Generators** headed by Prof. Z. Ismagilov were active in research under a number of problems:

♦ IR spectroscopy was used for studying the nature of sulfate complexes formed upon hydrogen sulfide adsorption on the surface of oxide catalysts. It has been shown that at temperatures > 100^oC the quantity of sulfates with the absorption bands at 1100 cm^{-1} decreases. This process is accompanied by simultaneous generation of sulfate groups characterized by high-frequency adsorption bands at 1260 cm^{-1} on the surface of the catalyst.

These sulfate groups were shown to be active in reaction of hydrogen sulfide oxidation. Reaction of hydrogen sulfide with sulfate groups leads to the decrease of their quantity and simultaneous elemental sulfur and water production.

The mechanism of direct partial oxidation of hydrogen sulfide over oxide catalysts was suggested which involves formation of sulfate-sulfite complexes at the initial stage, which then react with hydrogen sulfide from the gas phase or with physically adsorbed hydrogen sulfide to produce elementary sulfur and water.

♦ High-temperature methane decomposition over $Ni\text{-}Cu\text{-}Al_2O_3$ catalysts was studied in temperature range 625-675°C and P = 1 bar to produce hydrogen and catalytic filamentous carbon (CFC) with unique microstructure. It has been revealed, that the quantity of carbon production can reach 500 g/g cat at $T=625^oC$ over the catalyst containing 15 mass. % copper. $Ni\text{-}Cu\text{-}Al_2O_3$ catalysts prepared by coprecipitation were studied by X-ray and electron microscopy methods. The CFC texture and structure were characterized using X-ray, TEM and adsorption methods. Copper was established to be not only cross-linking additive, but stabilizing as well.

♦ Methods for preparation of monolithic supports based on titanium dioxide and aluminosilicate-based monoliths were developed. Introduction of Ca- and Na-montmorillonites as binding agents into the extruded material allows the plastic properties of the materials to be remarkably improved, the absence of drying-induced defects and a high mechanical strength to be provided.

A method for synthesis of impregnated magnesium-containing catalysts based on titanium oxide monolith support was developed. Experimental dependencies of sorption capacity to hydrogen sulfide and of catalytic activity to decomposition of ammonia on concentrations of magnesium, modifying agent and calcination temperature were established. The obtained experimental data were used for optimization of the composition of the impregnated magnesium-containing catalysts to be used for the processes of combined cleaning of gases from hydrogen sulfide and ammonia.

♦ The effects of ceria concentration and the sequence of supporting the active component and promoter on the activity of iron oxide catalysts supported on fiber materials were studied. Introduction of ceria was shown to allow the concentration of the active component to be decreased at the preserved catalytic activity to complete oxidation of propane. Optimal preparation conditions and catalyst composition were chosen.

♦ The influence of MgO concentration and temperature of thermal treatment of the support on the activity and stability of nickel catalysts was studies. The catalyst properties were found to depend on the magnesium concentration and temperature of thermal treatment of the promoted supports. An increase in the promoter concentration (to 13% of MgO) resulted in an increase in the catalytic activity of reduced nickel. In this case elevation of the thermal treatment temperature did not cause a change in the catalytic activity but a decrease in the catalyst resistance to coke formation.

♦ Modification of Cu-ZSM-5 catalysts with titanium was shown to enhance the stability to poisoning with sulfur compounds (H_2S) at 500°C. Some decrease in the activity observed upon sulfur poisoning at 400°C disappeared after the catalyst regeneration. Introduction of cerium promoters in the prepared catalysts allowed the catalyst stability in the presence of water vapor providing practically the same activity with water and without water at both 400 and 500°C.

♦ The composition of a monolithic Cu-zeolite catalyst modified simultaneously with titanium and cerium was proposed, the main catalyst components being in the washcoat. Testing of the catalyst demonstrated that it retained the activity for 20 hours in the presence of sulfur compounds and water impurities in the reaction mixture.

♦ Applicability of different kinds of reductants (hydrocarbons, CO, NH_3 and H_2S) for selective catalytic reduction of nitrogen oxides, as well as a possibility of activation of these molecules with ozone over typical DENOX catalysts was studied. Principal feasibility of reduction of nitrogen oxides by hydrogen sulfide was discovered. Hence, development of a technology for mutual neutralization of toxic H_2S and NO_x in technological waste gases seems realistic.

♦ Mn-Al-O catalysts were prepared based on alumina comprising χ–Al_2O_3, modified with Mg, La or Ce and calcined at 1300°C. They were found to be more stable and active against the catalysts based on χ-Al_2O_3 alone, including commercial catalysts ICT-12-40, and to retain their high activity when calcined at 1100°C for long period of time (20 hours). When used separately, the presence of χ–Al_2O_3 in the support and modification of γ-Al_2O_3 with the enumerated promoters did not provide the desired performance. The observed modifying effect is probably due to the components interaction in the presence of χ–Al_2O_3 and modifying agents to form high-temperature Mn and Al compounds (for example, hexaluminates of various composition) providing the high activity and stability of the modified Mn-Al-O catalysts. Thus, they can be recommended for high-temperature oxidation processes.

A joint research program for development of the technology for destruction of mixed organic wastes at Seversk (former Tomsk-7), contaminated with enriched U, isotopes of Pu and fission products has been carried out by the **Group of Direct Catalytic Hydrogen Sulfide Oxidation** headed by Dr. Mikhail A. Kerzhentsev with participation of the Institute of Technical Chemistry of the Ural Branch of RAS and the Siberian Chemical Complex in Seversk. For the treatment of these wastes a process of oxidation in catalytically active molten salts was proposed.

The studies of oxidation of individual organic compounds: saturated and aromatic hydrocarbons, alcohols, N and Cl containing compounds and waste components: tributyl phosphate, kerosene, vacuum pump oil, etc in alkaline metals carbonate melts have shown high efficiency of the process (over 99.99%) at relatively low temperatures 750-850°C. Under these conditions formation of NO_x is suppressed and main reaction products are CO_2 and H_2O. The effects of process parameters: space velocity, temperature, oxygen excess coefficient, and melt composition on the process efficiency were studied. Basing on these results an experimental installation for study of destruction of real U and Pu containing wastes in molten salts has been designed and fabricated in Tomsk-7, and experimental study of waste treatment in this installation was started.

A study of the oxidation of liquid rocket propellant unsymmetrical dimethylhydrazine (UDMH) has been carried out in the laboratory setup over a series of solid catalysts: $Cu_xMg_{1-x}Cr_2O_4/Al_2O_3$, Fe_2O_3/Al_2O_3, Pt/Al_2O_3, Pd/Al_2O_3, Ir/Al_2O_3, Cu/(ZSM-5) etc. The reaction intermediates were identified and a possible mechanism of UDMH catalytic oxidation has been suggested. The temperature dependencies of various product yields have been studied. The catalysts and process conditions for achieving the complete oxidation of UDMH to CO_2 and water with minimal concentrations of nitrogen oxides were selected.

On the basis of the research on catalytic oxidation of UDMH a process diagram and technical requirement for UDMH catalytic destruction has been developed. The process is based on the combination of UDMH catalytic fluidized bed oxidation and liquid phase catalytic oxidation of trace amounts of UDMH captured in scrubber liquids. Technical Design of the pilot installation for UDMH catalytic destruction with a capacity of 2 kg/h have been elaborated. State Rocket Center (SRC) “Academician V.P. Makeyev Design Bureau” in Miass has prepared detailed design documentation for the fabrication and assembly of the experimental installation. All the units of the installation have been constructed and the installation has been assembled at SRC and prepared for the start up and testing.

The proposed UDMH treatment technology is expected to solve the following problems: 1) utilization of UDMH directly at the rocket bases using mobile plants; 2) destruction of the wastes containing UDMH, for example, rinsing fluids after cleaning tanks for UDMH; 3) liquidation of the consequences of UDMH spills in emergency situations.

Two systems of Co-containing catalysts were under the study at the **Laboratory of Catalytic Conversion of Carbon Oxides** headed by Prof. T. Yurieva: Co hydrosilicates and Co-Al hydrotalcites. The main focus of studies was the nature of the cobalt species interaction with the silicon (or aluminum) containing oxide phase for both untreated samples and the samples after their treatment in the inert gas flow and the hydrogen flow.

The model system of *Co hydrosilicate* (stevensite-like structure) was thoroughly studied by a set of physical methods in respect of the evolution of its structure and physico-chemical properties during the treatments in the inert gas medium and hydrogen. DTG-DTA, FTIR, XRD, UV-Vis spectroscopy data were obtained. The results allowed to review the existing in literature data on the Co/SiO_2 catalysts and to conclude that the main route of chemical interaction of the Co cations with SiO_2 during preparation of Co/SiO_2 catalysts is Co-stevensite formation. Formation of Co-stevensite occurs every time when the pH of maternal solution exceeds 4.

The further studies showed, that Co^{2+} readily substitutes Mg^{2+} and Zn^{2+} in the stevensite structure. The cobalt reduction extent at 500˚C for the samples comprising *cobalt supported by Mg (or Zn) stevensite* is about 60-80 %. The catalytic properties of the metallic cobalt are significantly different from those of “normal” Co°. The metal-support interaction effect was supposed.

The *hydrotalcites of Co-Al*, and the samples comprising Co supported by Zn-Al and Mg-Al hydrotalcites were studied. The transformation of hydrotalcite-type structure into Me^{2+} aluminate during calcination proceeds gradually through an inverted spinel structure with a composition of $(Me^{2+}{}_{1-x}Al^{3+}{}_{x})(Me^{2+}{}_{x}Al^{3+}{}_{2-x})O_{4-2y-z}(OH)_{2y}\,(CO_3^{2-})_z$. Spinel phase structure inversion is supposed to be thermodynamically favorable owing to the presence of some anionic admixtures. Reduction of Co^{2+} species, located in the octahedron sites of inverted spinel phase (support), occurs at 580-620°C, and is accompanied by anionic admixtures removal from the spinel structure.

Reduction temperature strongly affects the catalytic properties of Co-Al catalysts in CO hydrogenation. Catalytic properties of Co-Al catalysts reduced at 600°C are similar to those, expected for the dispersed Co° particles according to the literature data. The catalytic properties of the Co-Al catalysts reduced at 470°C-480°C are dramatically different from those of same catalysts reduced at 600°C. A miserable specific activity, and an abnormally high selectivity towards olefins, including (surprisingly) ethylene, are characteristic for these samples.

Further XPS studies and FTIR studies of adsorbed CO molecules allowed us to propose the existence of the *metal-support interaction for Co-Al samples reduced at 470-480˚C*. The observed effect may by caused by localization of positive charge at metallic Co particles due to decoration of these particles by negatively charged nano-scale clusters of the Al-containing oxide.

The **Group of Reactions of Oxidation on Metals** headed by Prof. A. Khasin has detected two essentially different species of hydrogen adsorbed on a copper-zinc oxide catalyst $Cu_{0.08}Zn_{0.92}O$ pre-reduced by hydrogen (the model catalyst for methanol synthesis) at the range from room temperature to 493 K. A low energy of the chemisorption bond is characteristic of the first one, which is formed in a considerable equilibrium quantity at high hydrogen pressures close to atmospheric. Species of the second type are more strongly bonded to the surface of the reduced catalyst; they are readily formed at the whole range of conditions under study, and the equilibrium is established between the adsorbed and gaseous hydrogen.

The rate of ethylene epoxidation on silver films prepared in vacuum was found to have a maximum at average surface coverage with oxygen. This result is in good agreement with earlier obtained for silver powder.

The main result of the **Group of Catalytic Synthesis of Oxygen-Containing Compounds** headed by Dr. G. Volkova is the development of catalytically active compositions based on acid cesium salts of P-W HPA for dimethyl ether carbonylation to methyl acetate without use of halogen-containing promoters. The obtained systems are 5-10 times more active than described in literature.

The **Group of Dynamics of Surface Transformations** headed by Dr. A. Simakov fulfilled the complex study of the surface copper species in supported copper-titania catalysts and studied the kinetics of reactions of selective reduction of NO by ammonia and methane oxidation by oxygen. It has been shown, that the chain type of surface copper species are most active in these reactions.

The nature of surface adspecies of acetone oxime - key intermediate in the reaction of selective reduction of NO with propane - with surface centers of zeolite ZSM-5 ion exchanged with copper ions has been revealed.

DEPARTMENT OF HOMOGENEOUS AND COORDINATION CATALYSIS

HEAD OF THE DEPARTMENT PROF. VLADIMIR A. LIKHOLOBOV

Laboratory of Catalysis by Complex Metal Compounds
Head: Prof. Vladimir A. Likholobov

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

Laboratory of Catalytic Polymerization
Head: Prof. Vladimir A. Zakharov

Group of Synthesis of Surface Compounds
Head: Dr. Vladimir L. Kuznetsov

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

Group of Catalysts on Carbon Supports
Head: Prof. Vladimir A. Semikolenov

Researchers from the **Laboratory of Catalysis by Metal Complexes** headed by Prof. V. Likholobov concentrated their efforts on the following directions:

Development of synthetic methods, study and application of heteropoly compounds in catalytic processes and for catalyst preparation.

Possibility of synthesis of heteropoly acids with the low charge of the anion has been studied and new acid of this type, presumably, $H_4S_2W_{18}O_{62}$, has been obtained. New catalytic systems based on platinum and heteropoly compounds have been synthesized and studied by means of IR-spectroscopy, ESCA, TEM and thermogravimetric methods. In particular, Pt-modified catalysts were prepared from $H_3PMo_{12}O_{40}$; most active in the oxidative processes were shown to be catalytic systems derived from P-Mo and P-Mo-V heteropolycompounds.

Investigation of mechanisms of homogeneous catalysis, study of formation of colloidal particles and investigation of modified metal catalysts.

Propionyl and propionyl-ethyl complexes of platinum have been synthesized and studied by NMR as possible intermediates in ethylene carbonylation. Method of synthesis of raft-like Ni(0) particles was developed; by X-ray methods, the process of formation and the structure of Ni, Co, Ni-Pd and Co-Pd colloids have been studied. New bi-functional catalysts $M–M'O_x/EO_y$ (M – metal of VIII group, $M'O_x$ – low-valent oxide of transition metal from III-VI group, EO_y – oxidic support) for the low-temperature hydrogenation of nitrogen have been prepared; promotion effect was shown to increase in the row: $Ln_2O_3<Y_2O_3<CeO_2$. Ni catalysts modified with B and Pd have been investigated in hydrodechlorination of polychlorinated organic compounds; introduction of palladium in the catalysts was shown to result in a sharp increase in catalytic activity and change in selectivity due to changes in mechanism of the catalytic process (appearance of new stages).

Development of preparation methods for new carbon materials and elaboration of preparation methods for carbon-supported catalysts with platinum metals.

By thermal decomposition of nitrogen-containing organics on metallic catalysts, new filamentous carbon materials with a high content of nitrogen have been obtained. Effect of composition of Ni-Fe, Ni-Cu and Ni-Co alloys on the yield and microstructure of catalytic filamentous carbon formed on such catalysts from methane at temperature up to 700^o C have been investigated; high thermal stability and effectiveness of Ni-Cu catalysts were shown; conditions for production of CFC-II with the yield up to 500 g/g cat. and specific surface up to 300 m^2/g have been found.

Investigation was performed of the factors influencing metal dispersion and metal distribution in the carbon-supported catalysts prepared from complexes of Ru and Pd; by a number of physical methods were shown that decrease in metal dispersion upon increasing temperature of the catalyst treatment is caused by sintering of Pd particles whereas Ru species retain their high dispersion. Some approaches to preparation of catalysts for olefin alkylation with isobutane (from transition metals and aluminum chloride) have also been tried.

The members of the **Group of Catalysts and Processes Based on Heteropoly Acids** headed by Prof. K. Matveev were focussed on the following problems:

♦ Composition of Mo-V-P heteropoly acids (HPA-*n*) was optimized for the use them as catalysts for selective oxidation of 2-methyl-1-naphthol (2M1N) into 2-methyl-1,4-naphthoquinone (menadione, MD), a semiproduct of synthesis of K vitamins. The reactions were conducted in two-phase systems comprising an aqueous solution of HPA-n and a 2M1N solution in an organic solvent (OS). The activity and selectivity of the catalysts increased with *n* (the number of vanadium atoms in HPA-*n*). The selectivity of HPA-*n* also depended on the nature of OS. The maximal productivity (7.9 g MD/l·h) and selectivity (89.7%) was observed with HPA-11 or HPA-12, formulated as $H_aP_xMo_yV_nO_b$ with $1 \leq x \leq 3$; $8 \leq y \leq 16$, and 2M1N in trichloroethylene as the solvent.

♦ Synthones were chosen for new methods to synthesize isophytol (IP), which is a part of a vitamin E molecule. Citral is one of synthones for preparation of IP. Synthesis of citral also is of importance for food industry, medicine and perfumery.

♦ New homogeneous catalysts were developed for oxidation of low olefins into carbonyl compounds. Catalysts Pd·Pc+HPA-*n* containing Mo-V-P heteropoly acid HPA-*n*, where $6 \leq n \leq 12$ and a complex of Pd with HPA-n were demonstrated to be highly effective for oxidation of low olefins (C_2–C_4) into carbonyl compounds. Complexes of HPA-n with palladium in the oxidized (Pd^{2+}) and reduced (Pd^o) states allowed the range of stability of Pd^{2+}-complex to be much widened (at the range of 1.0 to 0.79 V) compared to that of the free Pd^{2+} ion (oxidative potential of 1.0 to 0.95 V). High selectivity, stability were characteristic of the synthesized new catalysts. They revealed the activity and productivity 3-8 times as high as those of the catalysts used before.

The **Laboratory of Catalytic Polymerization** headed by Prof. V. Zakharov was active under the following main subject areas:

Determination of the number of active sites and of the constant of growth rate for ethylene polymerization over a vanadium-magnesium catalyst

The radioactive inhibitors (^{14}CO) method was used for determination of the number of active sites and of propagation rate constants during ethylene polymerization over high-active vanadium-magnesium catalysts. The obtained kinetic parameters were close to ones determined before for the titanium-magnesium catalyst prepared using a similar support. The effect of reversible deactivation of the vanadium-magnesium catalyst was studied for the case of the polymerization in the presence of hydrogen. An ingenious deactivation mechanism based on formation of ‘dormant’ sites preserving the vanadium-polymer bonds was suggested.

Study of composition, structure and thermostability of solid methylalumoxane (MAO) - the active component of the SiO_2/MAO support; search for new supports and methods for their activation to prepare supported metallocene catalysts for olefin polymerization

DRIFTS and mass-spectrometric techniques were used for investigation of the structure of solid MAO. Thermal stability and transformations of MAO were studied at the temperature range of 20 to 250°C (release of $AlMe_3$ and methane at 20 – 150°C at the preserved three-dimensional structure of MAO and MAO destruction at above 170°C to release methyl radicals, methane and methyl derivatives of aluminium). DRIFTS studies allowed the data to be obtained indicating that the 3D MAO molecule may involve a water molecule, which diffuses from the bulk of MAO to the surface and reacts with Al-Me bonds to release methane.

Adoption of a new method for controlling the size and density of particles of the supported titanium-magnesium catalyst (grafting method)

Factors determining the morphology of particles of a magnesium-containing support, which were prepared using the grafting method developed at the Laboratory, were revealed. The grafting method provides an increase in the size and density of particles due to deposition of the support material on particles of the substrate introduced additionally into the reaction medium. Under the established optimal conditions, the support particle size can be increased from 20 – 40 μm to 50 – 60 μm, and the density of catalyst particles and of the formed polypropylene particles also can be increased.

Studies of the morphology of polymers formed at the early stage of polymerization over supported catalysts in order to reveal extra potentialities of controlling the polymer particle morphology

Scanning electron microscopy was used for studying morphology of polypropylene (PP) particles formed at the early stage of polymerization (prepolymer) over catalysts with different particle size and porosity. It was established that the prepolymer morphology, the relation of it with the catalyst morphology, as well as morphology evolution while the polymer yield increased depended on the catalyst porosity. Morphologies of the prepolymer and target polymer also depended on the ratio of rates of active sites generation and formation of the polymer that could be controlled through prepolymerization conditions. The prepolymer morphology was found to depend on the nature of the monomer to be polymerized (PE, PP and copolymers of ethylene with propylene).

The **Laboratory of Sulfide Catalysts** headed by Prof. A. Startsev has been studied the chemical composition of new (Ni,W) and (Ni,Mo) catalysts, obtained through metal complexes with S-containing ligands by determination of hydrogen sulfide evolved upon reaching the steady state operation conditions. Activity of the catalysts has been studied in model reaction of benzene hydrogenation. The results obtained demonstrate that the main regularities for these catalysts and catalysts prepared with the use of metal organic compounds are the same, whereas the developed method is simpler.

A novel method has been developed for preparation of supported over Al_2O_3 catalysts with the use of new molybdenum and tungsten metal complexes with S-containing ligands. The complexes are synthesized from water solutions, the initial compounds being molybdenum and tungsten oxides and elemental sulfur. The complexes were characterized by NMR, EXAFS and FTIR technique.

The **Group of Catalysts on Carbon Supports** headed by Prof. V. Semikolenov has studied the kinetic regularities of following reactions:

- Hydration of α-pinene into the mixture of *cis*- and *trans*-pinane;
- Selective oxidation of pinane into pinane hydroperoxide;
- Selective hydrogenation of pinane hydroperoxide to pinanol (mixture of *cis*- and *trans*-isomers).

DEPARTMENT OF EXPLORATORY AND APPLIED INVESTIGATIONS

HEAD OF THE DEPARTMENT PROF. BAIR S. BAL'ZHINIMAEV

Center for Catalysts Characterization and Testing
Head: Prof. Bair S. Bal'zhinimaev

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

Group of Petrochemical Synthesis
Head: Dr. Vyacheslav N. Romannikov

Laboratory of Zeolites and Acid Base Catalysis
Head: Prof. Eugenii A. Paukshtis

Group of Oxidation Catalysis with Sulfur-Containing Compounds
Head: Dr. Galina A. Bukhtiyarova

The activities of the **Center for Catalysts Characterization and Testing** headed by Prof. B. Bal'zhinimaev were concentrated at:

Statistic simulation of adsorption processes and reactions on supported nanosized catalysts involving effects of spillover, lateral interactions between adsorbate and metal atoms, changes in shape and surface morphology catalyst particles

A model of a supported active component particle involving non-additive interactions between metal atoms was developed. Equilibrium forms of the supported active particle was calculated at different temperatures. It was shown that coalescence of closely arranged particles could occur at sufficiently high temperatures (~1100 K) when dispersing of the supported catalyst particles was observed.

While considering a model reaction, quantitatively and qualitatively different kinetic characteristics were established for case of the reaction $A+B_2$ proceeding according to the Langmuir-Hinshelwood mechanism on a supported catalyst particle involving morphological rearrangement of the catalyst surface and diffusion of adsorbed species through the support surface against the case of the reaction on the smooth surface of a bulk catalyst.

The influence of reversible dissociative adsorption on the equilibrium shape and morphology of the active particle surface was studied to show that an increase in the adsorbate-metal interaction energy resulted in adsorption-induced reshaping of the initial cubic (or semispherical) particles into conical ones, a pronounced "chess"-like structure (alternating vacancies and ridges) being characteristic of the surface fragments of the supported active metal particle.

Non-classical (statistical imitation) models of dimensional effects and self-organization processes in catalytic systems

For vanadium catalysts for sulfuric acid production, statistical lattice simulation of crystallization of the active component melt in slit-like and cylindrical pores was carried out. The melt was simulated as a three-dimensional lattice with local interaction between the cells and a kind of binuclear vanadium complex which could occur in each cell. The studies of behavior of the melt in finite-size pores demonstrated for both types of pores that the temperature break in the curve of lattice configuration energy vs. temperature was shifted towards higher temperatures at a decrease in the pores size (from 100 to 20 characteristic sizes of the binuclear vanadium complex). This phenomenon was less pronounced for the slit-like pores than for cylindrical pores with the width equal to that of the slit-like pore.

Kinetic relaxation and isotope-dynamic studies of reduction of NO with propane over fiberglass catalysts

Adsorptive capacity of catalyst Pt/fiberglass was studied by isotope-dynamic method using a label ($^{15}N^{18}O$). Analysis of response isotope curves showed the follows: 1) there was practically no adsorptive capacity with respect to NO, even though the oxygen exchange rate was high enough; 2) in the presence of oxygen, there was not only simple increase in the number of adsorbed particles involved in the exchange but also formation of oxidized surface NO_x

compounds, presumably nitrates, which were more strongly bonded to catalyst surface. To support the conclusion, NMR and IR data showed that these species were nitric acid or nitrate complexes depending on water content in the catalyst.

Experimental results on isotopic substitution using labeled oxygen $^{18}O_2$ argued very weak isotopic oxygen exchange between the catalyst and gas phase. That was though to mean an extremely low rate of O_2 adsorption on the catalyst, the adsorption being most likely to be in not dissociated but molecular mode.

Studies of the structure of active component and mechanism of action of sulfide catalysts for hydrodesulfurization

IR spectroscopy was used to study adsorption of NO, CO, thiophene molecules on Co-Mo/Al_2O_3 catalyst and, separately, on the Al_2O_3 support and individual supported sulfides Co/Al_2O_3 and Mo/Al_2O_3. Non-selective and practically equal adsorption was demonstrated for NO and thiophene in all the systems under study.

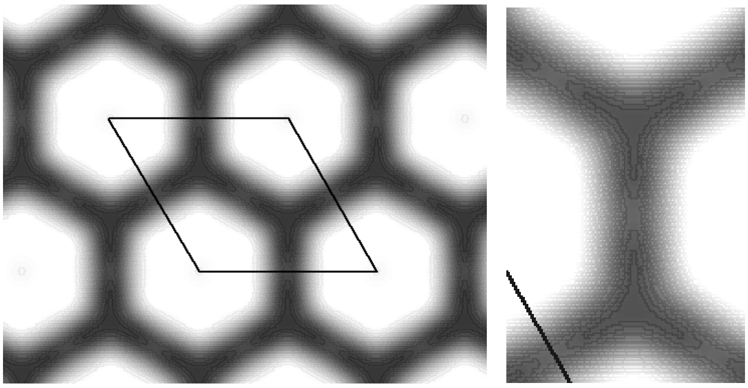
Data on adsorption of CO revealed that the charge state of Co atoms constituting the Co-Mo/Al_2O_3 catalyst differed from that in the bulky sulfide, i.e. cobalt atoms were in more oxidized state in the catalyst.

At the **Laboratory of Catalysts Activity Testing** headed by Dr. N. Bobrov a working model of a fundamentally new lab-scale kinetic installation was assembled for testing of activity of heterogeneous catalysts. A specific feature of the installation is the use of digital control of processes of preparation and separation of the initial reaction mixture. The development allows the productivity and accuracy of kinetic experiments to be enhanced and makes the operation more reliable at a lower cost and size.

Works on certification of dynamic adsorption devices fabricated under the BIC license are accomplished. The devices are used to determine specific surface area of disperse and porous materials in accordance to Russian and international standards. They are items of the State Instrument Registry.

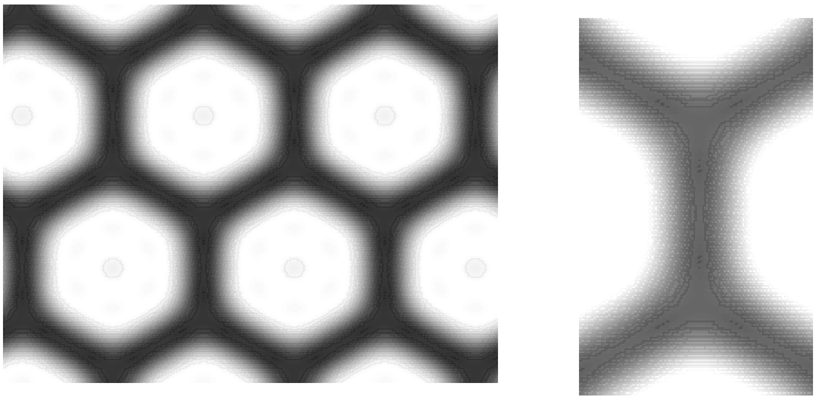
Intimate structure of hexagonal silicate mesostructures formed by different reaction pathways is studied in the **Group of Petrochemical Synthesis** headed by Dr. V. Romannikov. The relationship between the nature of electron density distribution in the inorganic wall, which are determined by pH of the medium during formation of silicate mesophases, and hydrostability of the mesostructure is established. Basic synthetic principles are developed for formation of silicate mesostructures in weakly acidic media that are the most prospective in view of preparation of mesostructured catalytic systems.

Mesostructure of silica prepared in alkali media (by S^+I^- pathway)

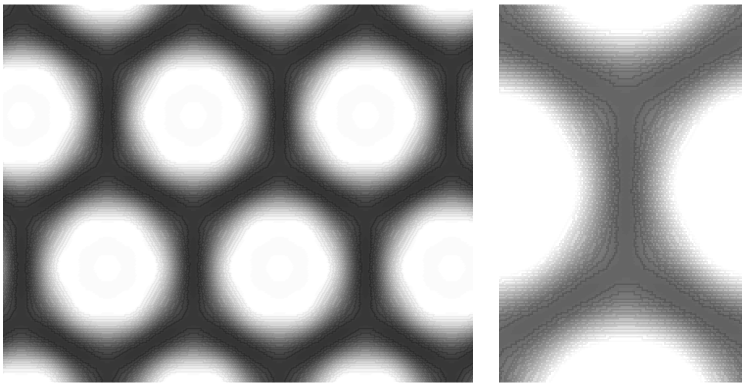


Electron density maps in typical mesostructures formed by different pathways in various media. Map fragments demonstrate differences in the structures of inorganic walls in the systems.

Mesostructure of aluminosilicate prepared in alkali media (by S^+I^- pathway)



Mesostructure of silica prepared in acidic media (by $S^+X^-I^+$ pathway)



The method of hydrothermal synthesis of Y-zeolites and ZSM-5 from various initial substances has been improved as a result of the work fulfilled by the **Laboratory of Zeolites and Acid Base Catalysis** headed by Prof. E. Paukshtis. Chemical composition, crystal structure and phase composition of obtained samples have been defined. The nature, strength and concentration of acid centers of H-zeolites with different extent of exchange to CO and N_2 have been studied.

The reaction of toluene chlorination has been studied in flow installation with tubular reactor and fixed catalyst bed over the series of zeolite catalysts, differ by structure, pore volume and nature of acid centers. Para- and orthotoluenes were the main products of the reaction. It has been revealed that zeolites with narrow pores and basic properties promote formation of para-substituted isomers.

IR diffuse reflectance spectroscopy (low-temperature CO adsorption as probe molecule at –50°C) has been used to study acidity of supports MAO/SiO_2 in supported metallocene catalysts for polymerization. It has been shown that activity of Cp_2ZrMe_2/MAO/SiO_2 catalysts correlates with the quantity of Lewis acid centers of definite strength.

IR spectroscopy (low-temperature CO adsorption as probe molecule at –110°C) has been used to investigate surface states of zirconium in supported active Cp_2ZrMe_2/MAO/SiO_2 catalysts and inactive Cp_2ZrMe_2/SiO_2 systems. An active in reaction of polymerization zirconium states are determined by CO implantation at 20°C.

The **Group of Oxidation Catalysis with Sulfur-Containing Compounds** headed by Dr. G. Bukhtiyarova proceeded with studying the regularities of generation of supported Fe-containing catalysts ($FeSO_4/SiO_2$; $Fe(NO_3)_3/SiO_2$) in temperature range 110-800°C by methods of Mössbauer spectroscopy, X-ray, IR spectroscopy, XPS.

DEPARTMENT OF CATALYTIC PROCESS ENGINEERING

HEAD OF THE DEPARTMENT PROF. ALEKSANDR S. NOSKOV

Laboratory of Kinetics of Catalytic Processes
Head: Dr. Sergei I. Reshetnikov

Group of Zeolites and Zeolite Based Catalysts
Head: Prof. Gennadii V. Echevskii

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

Laboratory of Dynamics of Catalytic Processes
Head: Dr. Andrey N. Zagoruiko

Laboratory of Unsteady-State Catalytic Methods for Gas Purification
Head: Prof. Aleksandr S. Noskov

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

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

Laboratory of Multiphase Processes Modeling
Head: Prof. Valerii A. Kirillov

Laboratory of Catalytic Processes in Dynamic Bed
Head: Prof. Gennadii G. Kuvshinov

The **Laboratory of Kinetics of Catalytic Processes** headed by Dr. S. Reshetnikov develops theoretical and experimental methods to study catalytic processes taking into account unsteady state of the catalyst.

An effect of time and temperature of V-Ti catalyst pretreatment with toluene on its activity and selectivity upon oxygen impacts was studied experimentally. The possibility to increase the yield of benzoic acid by increasing the time of catalyst treatment at high temperature has been shown.

Based on scheme of the reaction kinetics, an effect of chemical non-stationarity of two-path reaction has been studied. The model takes into account blocking up of one of two active sites by initial reagents.

Chromatographic method was used to measure the equilibrium values of benzene sorption, rates of sorption and desorption over ZSM-type zeolites in wide range of partial pressures and temperatures. Sorption equilibrium was shown to be in direct dependence on concentration of Brönsted acid sites.

Kinetic model was developed by the **Laboratory of Dynamics of Catalytic Systems** headed by Dr. A. Zagoruiko for the process of aromatization of the propylene-butylene fraction modeling and basic engineering of the process were accomplished.

Manufacturing of a semicommercial batch of the catalyst developed in the Laboratory for selective oxidation of hydrogen sulfide into sulfur to re-purify tail gases of Claus plants at the Omsk Oil Processing Plant was started.

The **Laboratory of Unsteady-State Catalytic Methods for Gas Purification** headed by Prof. A. Noskov carried out experimental and theoretical studies in the field of selective oxidation of nitrogen oxides over vanadium-containing catalysts. The results obtained allowed basic technological parameters to be determined and a catalytic reactor for treatment of industrial waste gases with low content of nitrogen oxides to be designed. The process is achieved by periodical reversing the flow of filtered gases through catalyst beds, ammonia as a reductant being fed in between the catalyst beds while unsteady-state processes of ammonia sorption of the vanadium-containing catalyst provide complete purification at variable volumes and compositions of the gas to be purified. Feeding and mixing units are arranged at the central part of the reactor to afford minimal heat loss.

A pilot installation based on this method for purification of waste NO_x gases from explosives production was assembled and started-up. Gas volumes fed to purification is 7,000 to 10,000 m^3. At the concentration of nitrogen oxides equal to 3 to 4 g/m^3 in the inlet gases, the residual NO_x concentration is not higher than 70 mg/m^3. Therefore, the purification efficiency is 98-99%. The process parameters (temperature, purification efficiency, reverse time) attained in practice are the same as calculated ones (jointly with the Laboratory of Industrial Catalytic Processes).

Temperature of inlet gases 15-20^{0}C

Gas output 7÷10 th. m^3/h

Catalyst V_2O_5/Al_2O_3

Catalyst loading 5 tons

Concentration of NO_x:

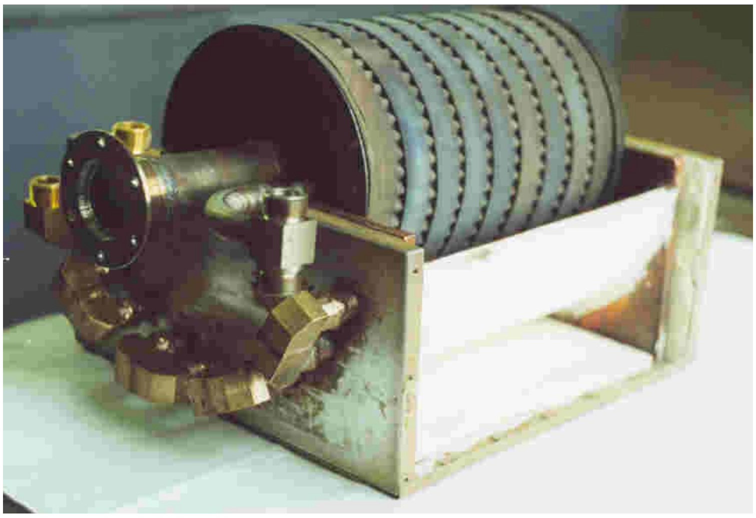
- **inlet 3-4 g/m^3**
- **outlet < 70 mg/m^3**

Separation efficiency from NOx >99%

Local mass transfer coefficients in a vented honeycomb catalyst were determined based on the developed NMR-tomographic method for measuring moisture content. The contactless method (MNR-tomography) was used for the first time to demonstrate that the mass exchange coefficients at the inlet of the honeycomb catalyst are 4-5 times as high as those of the outlet at the steady flow mode. A mathematical model of mass exchange between the flow and the solid phase inside the honeycomb catalyst was developed. The model allows the processes in the honeycomb catalysts to be described at a required accuracy that is of great importance to designing devices for neutralization of automotive exhaust gases, purification of flue gases etc.

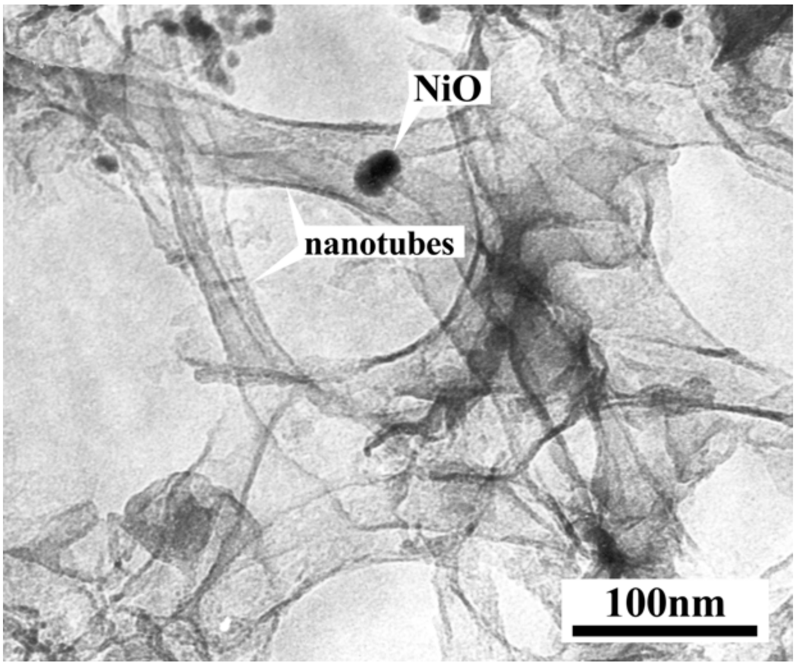
Numerical analysis of the phenomenon of heat wave propagation through a fixed catalyst bed in the course of consecutive reactions was carried out in the **Group of Mathematical Methods for Catalytic and Adsorption Processes Modelling** headed by Dr. N. Chumakova. The approach is based on a modified algorithm of orthogonal differential factorization which allowed the iterative strategy of constructing the autowave solution of nonlinear ordinary differential equations system to be optimized using simultaneous differential factorization from the opposite boundaries of the extending interval at every iteration step. The developed software makes it possible to determine effectively all the asymptotic parameters of a single heat wave (speed of propagation, maximal temperature, shift between concentration and heat fronts, etc.).A semicommercial evaluation unit of a self-contained heat-generating installation of up to 500 kWt capacity for catalytic combustion of coal and other kinds of solid fuels was designed at the **Laboratory of Catalytic Conversion of Solid Fuels and Wastes** headed by Dr. A. Simonov and tested. The catalytic combustion, if compared to the conventional methods, allows dimensions of fuel-combusting units to be considerably miniaturized and various kinds of solid fuels, including solid wastes, to be more effectively combusted.

A prototype of versatile self-contained heating systems (water heating boiler of 25 kWt capacity) was developed by the **Laboratory of Multiphase Processes Modeling** headed by Prof. V. Kirillov in cooperation with two defense enterprises. The systems allow ecologically sound combustion (catalytic oxidation) of natural gas. The provided level of ecological protection is superior to all of currently known device of this type.



A reinforced porous metal support and catalyst is developed for direct oxidation of natural gases in residential water heating system of 25 kWt capacity. It consists of Ni or Ti (65 wt %) + Al (30 wt %) and catalyst (5 wt %) 1%Pt/Al_2O_3 or 1%Pd/Al_2O_3.

Promising nanomaterials of the “solid air” type – silica aerogels comprising nickel oxide nanoparticles – were synthesized in the **Laboratory of Catalytic Processes in Dynamic Bed** headed by Prof. G. Kuvshinov without use of a laborious and very expensive method of drying from supercritical state. A high (higher than 1000 m^2/g) specific surface area, mesoporous structure (pore volume up to 5.6 cm^3/g) and high thermostability up to 900°C are characteristic of the aerogels. They were synthesized using the method of sol-gel templating of carbon nanofibers with silica reticular structures. Tetraethoxysilane was used as the source of silica, carbon being then burnt off. Structural analysis revealed the presence of silica nanotubes and nanofibers in the aerogels. The prepared aerogel was tried as catalyst for direct oxidation of hydrogen sulfide with molecular oxygen. It was shown to catalyze oxidation of hydrogen sulfide (0.5% in the mixture) into sulfur at 100% selectivity at 160°C in the presence of excess oxygen (up to 16% in the mixture). Sulfur was not accumulated on the catalyst under these conditions that provides long and stable catalyst operation.



DEPARTMENT OF CATALYTIC PROCESSES OF FINE ORGANIC AND BIOORGANIC SYNTHESIS

HEAD OF THE DEPARTMENT PROF. ALEKSANDR G. TOLSTIKOV

Group of Catalytic Synthesis of Biologically Active Compounds
Head: Prof. Aleksandr G. Tolstikov

Group of Liquid-Phase Catalytic Oxidation of Organic Compounds
Head: Prof. Zinaida P. Pai

The **Group of Catalytic Synthesis of Biologically Active Substances** headed by Prof. A. Tolstikov was focused on:

Reaction of catalytic asymmetric oxidation of model sulfides involving vanadium (V) peroxo complexes with chiral salicylaldemines were studied to improve optical yields of the produced sulfoxides.

General synthesis of optically active alkaloids of (-)-diptocarpamine (N-(isopropyl)-N′-(6-methylsulfinylhexyl)urea and (-)-ditocarpylidine (N,N′-bis(6-methylsulfinylhexyl)urea was accomplished using the method of *in situ* asymmetric oxidation of the sulfide precursors with hydrogen peroxide in the presence of vanadium (IV) complexes with chiral Shiff bases.

Catalytic activity and selectivity of new neutral complexes of ruthenium and rhodium with chiral ureas and thioureas synthesized from dehydroabietic acid and (S,S)-diphenylenediamine was studied with asymmetric reduction of acetophenone into optically active phenetyl alcohol through hydride transfer as an example.

Technological layout for synthesis of (±)-N-methyl-3-(*p*-trifluoromethylphenoxy)-3-phenylpropylamine, an active substance of psychotropic medications Phluoxetine and Prozak, was developed.

A simple technological procedure for synthesis of nucleosidemonophosphates was developed. Therefore, an ample and cheap enzyme alone, S′-nuclease (capable of hydrolyzing both RNA and DNA denatured by heating), can be substituted for such non-abundant enzymes as pancreatic and microbial nuclease and phosphodiesterases. The developed procedure makes the technology for synthesis of nucleosidemonophosphates much simpler and can be used for commercial production of these compounds.

The process for treatment of sulfite-bisulfite waste water to utilize sulfur dioxide in the form of the concentrated gas to be used for manufacturing of sulfuric acid was proposed by the **Group of Liquid-Phase Catalytic Oxidation of Organic Compounds** headed by Prof. Z. Pai for practical application at the Byisk Oleum Plant.

Kinetic regularities of desorption of sulfur dioxide from sulfite-bisulfite solutions were studied depending on the process conditions and mode. Conditions providing the optimal extraction of SO_2 were determined. The layout of the desorption stage was proposed and heat and mass balances were calculated for this stage.

OMSK DIVISION OF THE BORESKOV INSTITUTE OF CATALYSIS

Executive Director Vasilii S. Alfeev

Scientific Manager Prof. Valerii K. Duplyakin

SCIENTIFIC-RESEARCH SUBDIVISIONS

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

Group of Carbon Materials
Head: Dr. Georgii V. Plaksin

Laboratory of Catalytic Methods for Atmosphere Protection
Head: Prof. Pavel G. Tsyrul'nikov

Laboratory of Catalytic Processes
Head: Dr. Aleksandr S. Belyi

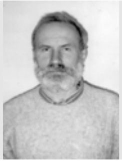
Laboratory of Kinetics and Modeling of Petrochemical Processes
Head: Prof. Nikolai M. Ostrovskii

Group of Zeolite-Containing Catalytst for Petrochemistry and Petroleum Refining
Head: Dr. Vladimir P. Doronin

SUBDIVISION OF PHYSICOCHEMICAL METHODS OF INVESTIGATION

Group of Adsorption
Head: Dr. Vladimir A. Drozdov

Group of X-Ray and Electron Microscopy Technique
Head: Dr. Aleksandr I. Nizovskii



Group of Spectral Methods
Head: Dr. Valentin P. Talzi

Analytical Group
Head: Tatiana V. Kireeva

DEPARTMENT OF EXPERIMENTAL TECHNOLOGY

HEAD: DR. ALEKSANDR I. ORUZHEINIKOV

DEPARTMENT OF APPLIED CATALYSIS

HEAD: KONSTANTIN V. KOLMOGOROV

SCIENTIFIC-RESEARCH SUBDIVISIONS

Members of the **Laboratory of Deep Petroleum Refining** headed by Prof. V. Duplyakin, including the **Group of Carbon Materials** headed by Dr. G. Plaksin are active under main subjects:

- Systemic approach to the design of catalysts of acidic action:

  - Supported oxides and sulfate-oxide composites (catalyst and the process of isobutane alkylation by butylenes)
  - Solid phosphorous acid on carbon supports (catalyst for butylenes oligomerization).

- Catalytic process and catalyst for olefins skeletal isomerization and oligomerization (jointly with the Laboratory of Kinetics and Modeling of Petrochemical Processes and Group of Zeolite-Containing Catalysts for Petrochemistry and Petroleum Refining).
- Development of new materials based on carbon and carbon containing composites including natural feedstock.
- Design of the technology for carbon molecular sieves production and processes of gas separation over sieves.

The research program of the **Laboratory of Catalytic Methods for Atmosphere Protection** headed by Prof. P. Tsyrul'nikov included:

- Development of catalysts for low temperature synthesis of ammonia over carbon support "Sibunit".
- Study of the nature of the high-temperature dispergation.
- Design of the catalyst "Cu/Sibunit" for methanol dehydrogenation to methylformate.

The **Laboratory of Catalytic Processes** headed by Dr. A. Belyi made a success in development of new generation of catalysts for oil hydrocarbon reforming and design of catalytic process for motor fuels production with the use of natural raw materials.

The research directions of the **Laboratory of Kinetics and Modeling of Petrochemical Processes** headed by Prof. N. Ostrovskii include:

- The theory and kinetics of catalysts deactivation
- Catalyst pellet design
- Kinetic methods for catalyst testing
- Reaction kinetics over new catalysts
- Chemical reactor modeling and optimization
- Development of computer programs.

The **Group of Zeolite-Containing Catalysts for Petrochemistry and Petroleum Refining** headed by Dr. V. Doronin is concentrated on the development and improvement of:

- Catalysts for catalytic cracking of petroleum fractions;
- Catalysts for the processes of diesel fuels hydrodeparaffinezation;
- Catalysts and supports based on natural clays and their intercalates.

SUBDIVISION OF PHYSICOCHEMICAL METHODS OF INVESTIGATION

The **Group of Adsorption** headed by Dr. V. Drozdov is engaged in systematic studies of physico-chemical principals of texture design for modern catalysts and adsorbents used for the processes of petroleum refining, petrochemistry and environment protection.

Texture and adsorptive properties of composites based on oxide systems and activated clays, modified zeolites placed in porous matrices of different chemical and phase composition are investigated intensively. The regularities of microstructure formation of carbon-carbonaceous materials, carbonaceous molecular sieves, obtained from plant feedstock are studied.

Application and development of numerical methods to obtain quantitative information about structural inhomogeneity of microporous objects of different composition and structure (carbon materials, zeolites, activated and intercalated clays) is among other directions of activities in the Group.

The **Group of Spectral Methods** headed by Dr. V. Talsi is engaged in NMR-spectroscopy of solutions and solid substances (Bruker AC 200P spectrometer) and IR spectroscopy study of catalyst surface.

The **Analytical Group** headed by T. Kireeva is focused on X-ray fluorescence analysis of solid substances (VRA-30 spectrometer), atomic absorption analysis (AAS-30 spectrophotometer) and traditional chemical and physico-chemical methods.

The Group is well equipped with modern physical devices, which allow one to perform the complete characterization of catalysts and supports, natural and technique water, diesel fuels, some biological objects, etc.

The experimental facilities of the **Group of X-Ray and Electron Microscopy Technique** headed by Dr. A. Nizovskii are:

X-ray analysis (diffractometers DRON-3, HZG-4/A);

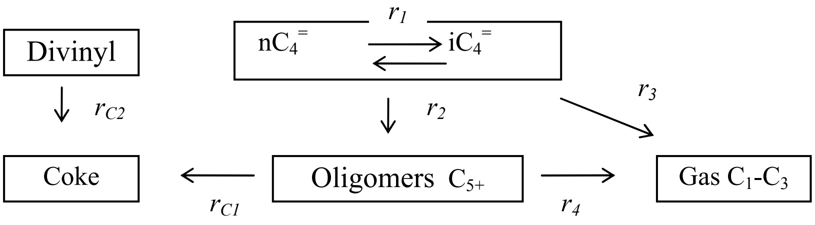
Electron microscopy (electron microscope BS-350).

MAIN ACHIEVEMENTS IN 2000

Kinetics of butylenes sceletal isomerization

The kinetic studying of industrially important process of isobutylene production with the subsequent synthesis of methyl-*tert*-butyl ether (MTBE) from isobutane and methanol are accomplished. Three types of the catalysts - Al_2O_3, F/Al_2O_3, Nb_2O_5/Al_2O_3 -were investigated.

The main reactions and products are:



The equations are obtained for main reactions – isomerization, oligomerization, disproportionation, cracking.

The reaction constants and activation energies are determined. The kinetic model is used for optimization of operating conditions of industrial reactor of ISOLENE process (the Laboratory of Kinetics and Modeling of Petrochemical Processes).

Kinetics of catalysts poisoning upon capillary condensation of reactants

Capillary condensation of some part of reactants in catalyst pores may have a considerable influence on the catalytic processes because of differences in the reaction kinetics and dynamics in liquid- and gas-filled pores. For hydrogen-based processes (hydrogenation, hydropurification), the low solubility of H_2 and other non-condensing components (H_2S) in the liquid phase is of importance. This is especially true for deactivation processes since H_2 behaves as an agent providing partial self-regeneration of the catalyst.

Experimental studies of the influence of capillary condensation on the nature of catalyst poisoning with sulfur (thiophene) were carried out with a model reaction of *p*-xylene hydrogenation as an example. 1%Pt/SiO_2 was used as the catalyst. Macroporous (KSK, $r_{ef}\approx10$ nm) and fine porous (KSM, $r_{ef}\approx3$ nm) supports provided the reaction both in gas phase (Pt/KSK) and under the conditions of capillary condensation (Pt/KSM).

It was established for the gas-phase reaction that poisoning was rapid and the kinetics independent of the catalyst. For the case of capillary condensation, the constant of poisoning rate was 1.6 – 2.0 times lower because the process was limited by diffusion in the liquid. The number of pulses resulting in complete catalyst poisoning changed depending on temperature and the occurrence of the capillary condensation (the Laboratory of Kinetics and Modeling of Petrochemical Processes)

Development of methods for determination (calculation) of textural parameters of porous materials of various compositions and structures based on adsorption structural method

A quantitative method was developed for restoring the function of micropore size distribution from experimental adsorption isotherms. The method was checked using both commonly known reference data on standard samples and the experimental data obtained with carbon, zeolite and clay materials (the Group of Adsorption).

Development of a new technology for processing of natural gas and oil fractions to produce motor fuels (Biforming process)

Experimental evidence of insertion of methane molecules into high-molecular products of higher alkane cracking was obtained. Typical catalysts for breakage of C-C bonds of higher hydrocarbons (acidified zeolites of various types) are inactive to coupled transformations of methane and higher alkanes. If the zeolites are modified with active components for dehydrogenation of C-H bonds of methane, they adopt fundamentally different bifunctional properties.

Catalytic properties of ZSM-5 zeolites modified with ions of Zn, Co, Ni, Mo, Sn and rare earth elements were studied in reactions of coupled transformation of methane and tetradecane. The nature of active sites of zeolites for dehydrogenation of C-H bonds was shown to have a considerable influence on the catalytic properties.

Interaction of methane with intermediates of tetradecane cracking was studies at 60 atm at the temperature range of 400-450°C. Two catalytic systems were discovered which provided the conversion of methane as high as 30-50% at the molar C_1/C_{14} ratio from 7 to 10. A total of C_{2+} hydrocarbon yield reached 115% on the basis of tetradecane fed to the reaction.

A pilot Biforming installation (for processing of 2.5 dm^3 of feedstocks a day) was assembled. Technological testing of the Biforming process was carried out using fractions of 98-175°C and *n*-butane. The process conditions were optimized using a commercial catalyst PR-51 to adopt them to commercial reforming process. If the feedstock to be processed contained *n*-butane fraction in amount of up to 10%, an increase in the yield of high-octane gasolines was shown to reach 4 to 6% due to transformation of C_3-C_4 hydrocarbons into typical components of motor fuels (aromatic and isoparaffin hydrocarbons). Life test of the PR-51 catalyst in the Bifroming process allowed no shorter than a year service cycle to be expected. Technical data were prepared for adoption of an existing industrial reforming installation for the Biforming process. The reconstruction of one industrial installation is expected to allow annual processing of 300,000 t of the gasoline fraction to increase production of high-octane components of motor fuels from 250 to 280-290 t (the Laboratory of Catalytic Processes).

Cycloalkane process for catalytic separation of C_1-C_4 hydrocarbon gases and hydrogen

A pilot two-reactor installation consisting of a reforming unit and a hydrogenation unit was designed, assembled and put into operation. Hydrogen-containing gas (HCG) is supplied to the hydrogenation reactor where hydrogen is transferred into cyclohexane hydrocarbons formed by hydrogenation at the rate equal to the rate of hydrogen generation in the reforming reactor. HCG is separated from liquid hydrogenation products and fed to the reforming reaction zone. Balance experiments were conducted for the process. The complete recycling of the hydrocarbon components of HCG into the reforming zone was established to be accompanied by transformations of C_3-C_4 hydrocarbons to form additional amounts of high-octane catalyzate. The catalyzate yield increased from 86.5 to 91%. This version of the process was shown to provide an increase in the selectivity at a considerable decrease in the yields of C_3-C_4 by-products (the Laboratory of Catalytic Processes).

Catalyst for skeletal isomerization of n-butylenes

The study deals with the problem of production of ecologically friendly high-octane gasolines in Russia. The annual production of octane-improving additive to gasoline, methyl-*tert*-butyl ester (MTBE) is to be increased from 300,000 to 3,000,000 t in the near future.

The ISOLEN process for isomerization of *n*-butylenes to isobutylene to be then subjected to esterification with methanol into MTBE was proposed based on the research accomplished in 1999. A catalyst for skeletal isomerization of *n*-butylenes was developed based on the "zirconia-alumina" system. The catalyst reveals a higher stability compared to that of the catalyst based on the "niobium oxide-alumina" system developed earlier (the Laboratory of Deep Petroleum

Refining, the Laboratory of Kinetics and Modeling of Petrochemical Processes, the Group of Zeolite-Containing Catalysts for Petrochemistry and Petroleum Refining).

Software

Mathematical models and necessary software were developed for the following processes:

- Regeneration of cracking catalysts;
- Dehydrogenation of isobutene into isobutylene;
- Skeletal isomerization of butylenes into isobutylene;
- Air drying using selective water sorbents (the Laboratory of Kinetics and Modeling of Petrochemical Processes).

ST. PETERSBURG DIVISION OF THE BORESKOV INSTITUTE OF CATALYSIS

DIRECTOR AND SCIENTIFIC MANAGER
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

St. Petersburg Division of the Boreskov Institute of Catalysis was founded in the beginning of 1999 in order to intensify R&D activities in the field of commercial processes for the synthesis of complex chemical products, polymers and polymeric composites using catalytic techniques, and to accelerate the commercialization of research results in the European region of Russia.

Research results

- Emulsion polymerization mechanism studies afforded revealing the approaches to the control over latex particle morphology and suggesting a new process for hollow particle latex synthesis.
- Peculiarities of ethylene polymerization and co-polymerization with higher α-olefins are studied using catalytic systems based on a series of metallocenes and metal-siloxanes.
- Kinetic features and mechanism of graft polymerization of some monomers onto polypropylene are studied.

RESEARCH ACTIVITY

OXYGEN ADSORPTION ON THE Ag(111) SURFACE: A QUANTUM CHEMICAL STUDY BY THE NDDO/MC METHOD

M.A. Milov, I.L. Zilberberg, S.Ph. Ruzankin, G.M. Zhidomirov

J. Molec. Catal. A: Chemical, 158 (2000) pp. 309-312.

The forms of the atomic oxygen adsorbed on the Ag(111) face were investigated using the semiempirical NDDO/MC method within the modified cluster approximation. Two oxygen positions - surface (over the octahedral hollow) and the subsurface (in the hollow) one - between the first two layers of (111) face were studied. A cross section of the potential energy for the oxygen penetration into subsurface positions has been computed. A new approach was applied to take into account the lattice relaxation caused by the interaction with adsorbate. The double-CI-like correlation corrections to the diffusion and desorption barriers were estimated. The barrier of the oxygen atom diffusion through the surface was shown to be substantially lower than that of the desorption.

OXYGEN DIFFUSION THROUGH THE Ag(111) SURFACE: A QUANTUM CHEMICAL STUDY BY THE NDDO/MC METHOD

M.A. Milov, I.L. Zilberberg, S.Ph. Ruzankin, G.M. Zhidomirov

J. Struct. Chem., 41 (2000) pp. 248-254.

The forms of the atomic oxygen adsorbed on the Ag(111) face were investigated using the semiempirical NDDO/MC method within the modified cluster approximation. Two oxygen positions - surface (over the octahedral hollow) and the subsurface (in the hollow) one - between the first two layers of (111) face were studied. A cross section of the potential energy for the oxygen penetration into subsurface positions has been computed. A new approach was applied to take into account the lattice relaxation caused by the interaction with adsorbate. The double-CI-like correlation corrections to the diffusion and desorption barriers were estimated. The barrier of the oxygen atom diffusion through the surface was shown to be substantially lower than that of the desorption.

ON THE PROBLEM OF DIFFERENTIATION OF ACETONE ADSORPTION SPECIES ON THE SILICA GEL: MOLECULAR MODELS OF ADSORPTION COMPLEXES

N.A. Kachurovskaya, G.M. Zhidomirov, Yu.I. Aristov

J. Molec. Catal. A: Chemical, 158 (2000) pp. 281-285.

In the framework of the cluster approach *ab initio* calculations of the adsorption complexes of acetone molecule with an isolated terminal OH group of silica gel (S1), with the fragment including hydrogen-bonded OH group (S2) and with two separated terminal OH groups simulating bifurcated acetone interaction (S3) were carried out. It is found that the difference between the stability of acetone complexes S1 and S2 is insignificant, and it is concluded that the bifurcated acetone interaction could result in a more stable adsorption form of acetone with silica gel.

ICOSAHEDRAL SYMMETRY STRUCTURES WITH OPEN-SHELL ELECTRONIC CONFIGURATION H^N (N = 1 - 9)

B.N. Plakhutin, R. Carbó-Dorca* (*Universitat de Girona Albereda, Girona, Spain)

Physics Letters A, 267 (2000) pp. 370-378.

A general structure of the states' energy levels has been derived for systems of icosahedral symmetry (I, I_h) having the degenerate open-shell electronic configuration h^N ($dimh = 5$; N = 1-9). Energies of the states have been derived in terms of the integral invariants $H^k(h,h)$ which are similar to the Slater-Condon parameters $F^k(l,l)$ for an atom with configuration l^N. Similar representations have been derived for electron repulsion integrals over the five-fold degenerate *h* orbitals. A discussion is presented about the relation between the energy spectra of the states for the configuration h^N under consideration and for the parent electronic configuration d^N of an atom.

OBSERVATION OF TWO PARAMAGNETIC SPECIES IN ELECTRON TRANSFER REACTIONS WITHIN CESIUM MODIFIED X AND Y ZEOLITES

R.I. Samoilova[a], A.A. Shubin, M.K. Bowman[b], J. Huttermann[c], S.A. Dikanov[a,d] ([a]Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia; [b]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, USA; [c]Universität des Saarlandes, Hamburg (Saar), Germany; [d]University of Illinois at Urbana-Champaign, Urbana, USA)

Chem. Phys. Lett., 316 (2000) pp. 404-410.

Tetrachloro-1,2-benzoquinone (o-chloranyl) has been used as a probe molecule to examine its interaction with catalytically active basic sites of cesium modified X and Y zeolites. Applying of CW and pulsed EPR it became possible to detect for the first time two paramagnetic species formed in the electron transfer reaction of active sites with o-chloranyl. One species is an anion-radical of o-chloranyl trapped in zeolite cage in the surrounding of alkaline ions. The other one is located in the zeolite lattice and comprises a center with a hole localized on oxygen(s) adjacent to the aluminum carrying about 50% of unpaired spin density.

ACTIVITY OF PEROXO AND HYDROPEROXO COMPLEXES OF Ti(IV) IN OLEFIN EPOXIDATION BY MONO AND BISPEROXO COMPLEXES OF Mo(VI): A DENSITY FUNCTIONAL MODEL STUDY

I.V. Yudanov, C. Di Valentin*, P. Gisdakis, N. Rösch**** (*Università degli Studi di Pavia, Pavia, Italy; **Technical University of Munich, Garching, Germany)

J. Molec. Catal. A: Chemical, 158 (2000) pp. 189-197.

Olefin epoxidation by Mo(VI) peroxo complexes was computationally investigated (DFT B3LYP) for various monoperoxo models $X_2MoO(O_2)(H_2O)(NH_3)$ with anionic ligands X and the experimentally known complex $MoO(O_2)(dipic)(H_2O)$. All these monoperoxo complexes exhibit higher barriers for direct oxygen transfer to ethylene than the reference bisperoxo complex $MoO(O_2)_2(H_2O)(NH_3)$ with the same base ligand configuration; the most electronegative ligands X induce the lowest barriers. A molecular orbital analysis reveals factors that govern the activity of the peroxo ligand and corroborates the electrophilic character of the attack of a peroxo group on the olefin.

OLEFIN EPOXIDATION BY PEROXO COMPLEXES OF Cr, Mo, AND W: A COMPARATIVE DENSITY FUNCTIONAL STUDY

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J. Org. Chem., 65 (2000) pp. 2996-3004.

The epoxidation of olefins by peroxo complexes of Cr(VI), Mo(VI) and W(VI) was investigated using the B3LYP hybrid density functional method. For the mono- and bisperoxo model complexes with the structures $(NH_3)(L)M(O)_{2-n}(\eta^2\text{-}O_2)_{1+n}$ (n = 0, 1; L = none, NH_3; M = Cr, Mo, W) and ethylene as model olefin, two reaction mechanism were considered, direct oxygen transfer and a two-step insertion into the metal-peroxo bond. The calculations reveal that direct attack of the nucleophilic olefin on an electrophilic peroxo oxygen center via a transition state of spiro structure is preferred as significantly higher activation barriers were calculated for the insertion mechanism than for the direct mechanism. W complexes are the most active in the series investigated with the calculated activation barriers of direct oxygen transfer to ethylene decreasing in the order Cr > Mo > W. Barriers of bisperoxo species are lower than those of the corresponding monoperoxo species. Coordination of a second NH_3 base ligand to the mono-coordinated species, $(NH_3)M(O)_2(\eta^2\text{-}O_2)$ and $(NH_3)MO(\eta^2\text{-}O_2)_2$, results in a significant increase of the activation barrier which deactivates the complex. Finally, based on a molecular orbital analysis, factors that govern the activity of the metal peroxo group $M(\eta^2\text{-}O_2)$, in particular the role of metal center are discussed.

STRUCTURAL TRANSFORMATIONS IN OVERLAYER AND STICKING PROBABILITY DURING CHEMISORPTION: OXYGEN ON (100) SURFACE OF METALS

A.N. Salanov, V.N. Bibin, V.T. Yakushko

J. Molec. Catal. A: Chemical, 158 (2000) pp. 367-372

The effect of the formation of p(2x2) and c(2x2) adsorption structures on the O_2 sticking probability was studied by the simulation of the O_2 chemisorption on a (100) metal surface. The model used in the simulation took into account direct and indirect adsorption pathways and lateral interactions in the adsorption layer. The ratio between the activation energy of adsorption via the direct and indirect pathways (E_{dir}/E_{indir}) determines the character of the structural transformations in the adsorption layer, which, in turn, determines the S(θ) dependence. The direct pathway predominates at $E_{dir}/E_{indir}<7-8$. In this case Langmuir adsorption is observed, and S smoothly decreases with the θ growth. The indirect pathway predominates at $E_{dir}/E_{indir}>7-8$. In this case the island-mediated adsorption is observed and the S(θ) dependence has a maximum.

Monte-Carlo Simulation to Study Physico-Chemical Processes

KINETICS OF DISSOCIATIVE ADSORPTION ON STEPPED SURFACES OF PLATINUM

V.I. Savchenko, N.I. Efremova

Kinetics & Catalysis, 41 (2000) pp. 127-131.

The kinetics of dissociative adsorption of oxygen was studied by the Monte Carlo method for a model which supposed that absorption occurs with a high rate only on steps and that O_{ads} may migrate from steps onto terraces and backward. At the relatively low activation energy of diffusion from steps onto terraces E_{dif} ~ 75 kJ/mol (E_{dif} is lower by 4 kJ/mol in the back direction), the function lg(s(Θ)), where *s* is the sticking coefficient and Θ is the surface coverage by oxygen atoms, is almost linear at 300 K; that is, the Roginskii–Elovich adsorption equation is obeyed. If it is supposed that the bonding energy of adatoms on terraces is slightly higher than that on steps, and the sticking coefficient is constant and equal to s_0 up to high degrees of coverage as well as in the model of the kinetics of adsorption with a precursor state.

MATHEMATICAL MODELING OF WAVE PHENOMENA IN THE OXIDATION OF CO ON THE Pt(100) SURFACE

N.I. Efremova, V.I. Savchenko

Kinetics & Catalysis, 41 (2000) pp. 633-638.

CO oxidation on Pt(100) is studied by the Monte Carlo method using a model that accounts for the phase transition (1 × 1) ↔ (hex). The influence of surface diffusion of CO_{ads} on the velocity of wave propagation of O_{ads} and CO_{ads} and the distribution of the species in the reaction zone is studied.

THE ROLE OF SUBSURFACE OXYGEN IN OSCILLATORY BEHAVIOR OF $CO+O_2$ REACTION OVER Pd METAL CATALYSTS: MONTE CARLO MODEL

E.I. Latkin*, V.I. Elokhin, A.V. Matveev, V.V. Gorodetskii (*Novosibirsk State University, Novosibirsk, Russia)

J. Molec. Catal. A: Chemical, 158 (2000) pp. 161-166.

The statistical lattice model constructed for $(CO+O_2)$/Pd reaction takes into account the change of surface properties due to the penetration of the adsorbed oxygen into subsurface layer. The model demonstrates the oscillations of the rate of CO_2 formation and the concentrations of the adsorbed species. Autowave processes on the model palladium surface accompany these oscillations. The determining role of the diffusion intensity and the lattice size on the synchronization and stabilization of surface oscillations has been revealed. The existence of the reaction zone between the moving adsorbate islands characterised by the elevated concentration of the free active centres has been shown. The results obtained make possible to interpret the surface processes on the atomic scale.

SURFACE RESTRUCTURING AND APERIODIC KINETIC OSCILLATIONS IN HETEROGENEOUS CATALYTIC REACTIONS

V.P. Zhdanov

Physica D, 144 (2000) pp. 87-96.

The paper contains Monte Carlo simulations of kinetic oscillations, chaos and pattern formation in NO reduction by hydrogen on Pt(100) in the framework of the model taking into account NO-induced restructuring of the catalyst surface.

MODEL OF OSCILLATORY PATTERNS IN CELLS: AUTOCATALYSIS AND TRANSPORT VIA THE CELL MEMBRANE

V.P. Zhdanov

Phys. Chem. Chem. Phys., 52 (2000) pp. 5268-5270.

The paper contains simulation of oscillatory patterns in cells in the framework of the model taking into account autocatalysis in the cytoplasm and transport via the cell membrane.

SIMULATION OF THE KINETICS OF OXIDATION OF SATURATED HYDROCARBONS ON Pt

V.P. Zhdanov[1,2], B. Kazemo[1] ([1]Chalmers University of Technology, Göteborg, Sweden; [2]Boreskov Institute of Catalysis, Novosibirsk, Russia)

J. Catal., 195 (2000) pp. 46-50.

The steady-state kinetics of C_3H_8 oxidation on Pt are calculated assuming the process to be limited by concerted dissociative adsorption of C_3H_8 on vacant sites near adsorbed oxygen atoms (with breaking of a C-H bond and formation of OH). The results, obtained by using (1) the ideal model implying Langmuir adsorption, (2) a model based on the assumption that the saturation oxygen coverage is lower than one monolayer, and (3) a model taking into account adsorbate-adsorbate lateral interactions, indicate that the latter two models can reproduce the apparent reaction orders with respect to C_3H_8 and O_2, observed experimentally under the lean-burn conditions. Model 3 is preferable because its basis is physically more sound.

SIMULATIONS OF DESORPTION FROM AMORPHOUS FILMS

V.P. Zhdanov, **P.R. Norton*** (*University of
Western Ontario, London, Canada)

Surf. Sci., 459 (2000) pp. 245-255.

The structure of amorphous films formed at low temperatures is characterized by an abundance of unconnected bonds and/or topological disorder associated with variation in the number of particles forming elementary cells. Desorption from such films, occurring at higher temperature, may be complicated by film crystallization resulting from diffusion of particles. The first Monte Carlo simulations explicitly treating the interplay of all these processes is presented. The desorption from thin porous two-dimensional lattice films (up to 100 monolayers) generated by using the ballistic-deposition rules is analyzed. Employing various schemes of diffusion of particles in the film, it is demonstrated that for the model under consideration the desorption rate is initially high, but then it rapidly drops and further on becomes nearly constant, i.e. the apparent order of the desorption kinetics is close to zero.

GROWTH OF AMORPHOUS FILMS AT LOW TEMPERATURES: THE ICE MODEL

V.P. Zhdanov, **P.R. Norton*** (*University of
Western Ontario, London, Canada)

Surf. Sci., 449 (2000) L228-L234.

The paper presents Monte Carlo simulations of the growth of an amorphous ice films on the uniform substrate at low temperatures. The employed 1+1 lattice model takes into account anisotropy of interactions between water molecules. In addition, the newly arrived molecules are allowed to relax. The time dependence of the interface width is found to be described by power law with exponent β=0.28-0.30, typical for the conventional ballistic deposition models. This finding supports the concept of universality of the growth of amorphous interface.

KINETICS OF THIN OXIDE FILM GROWTH ON METAL CRYSTALS

V.P. Zhdanov, **P.R. Norton*** (*University of
Western Ontario, London, Canada)

Surf. Rev. Lett., 7 (2000) pp. 135-139.

The paper contains modifications of the Mott-Cabrera theory of the kinetics of thin oxide film growth on metal crystals.

CHAIN LENGTH SCALING OF PROTEIN FOLDING TIME: BETA SHEET STRUCTURES

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([1]Chalmers University of Technology, Göteborg,
Sweden; [2]Boreskov Institute of Catalysis,
Novosibirsk, Russia)

J. Chem. Phys., 113 (2000) pp. 883-890.

It is presented comprehensive 3D lattice Monte Carlo simulations of the folding kinetics of two-turn antiparallel β sheets. The model employed takes into account isotropic nonspecific interactions as in previous flexible heteropolymer models and also orientation-dependent monomer–monomer interactions, mimicking the formation of hydrogen bonds and chain rigidity. The chain length is varied from N = 15 to 33. For each chain length, the fastest folding temperature, T_{fast}, folding temperature, T_{fold}, and glass-transition temperature, T_g are calculated. The time-averaged occupation probability of the native state is found to be nearly independent of N at all temperatures. The dependence of T_{fast} and T_{fold} on N is accordingly relatively weak. The temperature interval where the folding is fast rapidly decreases with increasing N. For the chain lengths chosen, T_{fold} slightly exceeds T_g. The dependence of the folding time τ_f on N is well fitted by using the power law, $\tau_f \propto N\lambda$. The exponent λ is found to depend on temperature and on the distribution of nonspecific interactions in the chain. In particular, λ=2.7–4.0 at $T = T_{\mathrm{fast}}$ and 5.2 at T slightly below T_{fold}. Evaluating τ_f in real units at T near T_{fold} yields physically reasonable results.

SIMULATION OF DIFFUSION OF VESICLES AT A SOLID-LIQUID INTERFACE

V.P. Zhdanov[1,2], **B. Kazemo**[1] ([1]Chalmers University of Technology, Göteborg, Sweden; [2]Boreskov Institute of Catalysis, Novosibirsk, Russia)

Langmuir, 16 (2000) pp. 4416-4419.

The paper contains Monte Carlo simulations of diffusion of vesicles at a solid-liquid interface.

SIMULATION OF ADSORPTION KINETICS OF LIPID VESICLES

V.P. Zhdanov[1,2], **C.A. Keller**[1], **K. Glasmästar**[1], **B. Kasemo**[1]([1]Chalmers University of Technology, Göteborg, Sweden; [2]Boreskov Institute of Catalysis, Novosibirsk, Russia)

J. Chem. Phys., 112 (2000) pp. 900-909.

Employing the Monte Carlo technique, the kinetics of vesicle adsorption at a solid–liquid interface has been studied. The proposed model combines a treatment of the surface kinetics, including spontaneous, adsorption- and lipid-membrane-induced decomposition of adsorbed vesicles, and limitations of the adsorption rate by vesicle diffusion in the solution. With this model, different kinetic cases, corresponding to various scenarios of vesicle adsorption and decomposition, have been demonstrated. The general results are employed to simulate recent experimental kinetic data for adsorption of small phospholipid vesicles at a SiO_2 surface.

DIFFUSION-LIMITED KINETICS OF VESICLE GROWTH

V.P. Zhdanov[1,2], **B. Kazemo**[1] ([1]Chalmers University of Technology, Göteborg, Sweden; [2]Boreskov Institute of Catalysis, Novosibirsk, Russia)

Langmuir, 16 (2000) pp. 7352-7354.

The paper contains the theory of diffusion-limited kinetics of vesicle growth.

FORMATION OF SUPPORTED MEMBRANES FROM VESICLES

C.A. Keller, K. Glasmästar, **V.P. Zhdanov**[1,2], **B. Kazemo**[1] ([1]Chalmers University of Technology, Göteborg, Sweden; [2]Boreskov Institute of Catalysis, Novosibirsk, Russia)

Phys. Rev. Lett., 84 (2000) pp. 5443-5446.

Using a combination of the quartz crystal microbalance and surface plasmon resonance techniques, the spontaneous formation of supported lipid bilayers from small (~25 nm) unilamellar vesicles has been studied. Together these experimental methods measure the amount of lipid adsorbed on the surface and the amount of water trapped by the lipid. With this approach, for the first time, it became possible to observe in detail the progression from the adsorption of intact vesicles to rupture and bilayer formation. Monte Carlo simulations reproduce the data.

ORDERING OF ADSORBED PROTEINS

V.P. Zhdanov[1,2], **B. Kazemo**[1] ([1]Chalmers University of Technology, Göteborg, Sweden; [2]Boreskov Institute of Catalysis, Novosibirsk, Russia)

Proteins, 40 (2000) pp. 539-542.

The paper contains Monte Carlo simulations of ordering of adsorbed proteins.

MONTE CARLO SIMULATION OF DIFFUSION OF ADSORBED PROTEINS

V.P. Zhdanov[1,2], **B. Kazemo**[1] ([1]Chalmers University of Technology, Göteborg, Sweden; [2]Boreskov Institute of Catalysis, Novosibirsk, Russia)

Proteins, 39 (2000) pp. 76-81.

The paper contains Monte Carlo simulations of diffusion of adsorbed proteins.

STANDING CHEMICAL WAVES IN BISTABLE REACTIONS ON COMPOSITE CATALYTIC SURFACES

V.P. Zhdanov[1,2], **B. Kazemo**[1] ([1]Chalmers University of Technology, Göteborg, Sweden; [2]Boreskov Institute of Catalysis, Novosibirsk, Russia)

Phys. Rev. B, 62 (2000) R4849-R4852.

Using as an example the $2A + B_2 \rightarrow 2AB$ reaction occurring via the standard Langmuir-Hinshelwood mechanism, it has been shown by Monte Carlo simulations that the shape of the standing fronts, which can be observed in bistable reactions at the surface of a catalyst composed of two active metals, is crucially dependent on the energetics of adsorption on the metals forming a catalyst.

OSCILLATIONS AND CHAOS IN CATALYTIC REACTIONS ON THE NM SCALE

V.P. Zhdanov[1,2], **B. Kazemo**[1] ([1]Chalmers University of Technology, Göteborg, Sweden; [2]Boreskov Institute of Catalysis, Novosibirsk, Russia)

Physical Review E, 61 (2000) pp. R2184-R2187.

Monte Carlo kinetics of the $\mathrm{2A + B_2 \rightarrow 2AB}$ reaction occurring on a 20-30 nm-sized crystallite in the case when reactant adsorption on one of its facets results in surface restructuring is presented. The latter is described on the basis of the well-defined lattice-gas model predicting phase separation in the overlayer. Oscillatory and chaotic kinetic regimes are found in the simulations. The mechanism of kinetic chaos on the nm scale is shown to be unique compared to that proposed for reactions on single-crystal surfaces.

OSCILLATIONS IN CATALYTIC REACTIONS ON THE NM SCALE

V.P. Zhdanov

Catal. Lett., 69 (2000) pp. 21-25.

The Monte Carlo simulations of the oscillatory kinetics of CO oxidation on catalytic metals in the case when the reaction is accompanied by the formation of surface oxide are presented. The lattice size is varied from 50×50 to 3×3 in order to mimic nm catalyst particles. More or less regular oscillations are found for the sizes down to 15×15.

SIMULATIONS OF THE REACTION KINETICS ON NANOMETER SUPPORTED CATALYST PARTICLES

V.P. Zhdanov[1,2], **B. Kazemo**[1] ([1]Chalmers University of Technology, Göteborg, Sweden; [2]Boreskov Institute of Catalysis, Novosibirsk, Russia)

Surf. Sci. Rep., 39 (2000) pp. 25-104.

The paper contains a review of simulations of the reaction kinetics on nanometer supported catalyst particles.

CATALYSIS IN THE NM-REGIME: MANUFACTURING OF SUPPORTED MODEL CATALYSTS AND THEORETICAL STUDIES OF THE REACTION KINETICS

B. Kasemo*, S. Johansson*, H. Persson*, P. Thormahlen*, V.P. Zhdanov (*Chalmers University of Technology, Göteborg, Sweden)

Topics in Catal., 13 (2000) pp. 43-53.

The paper briefly reviews the methods employed to fabricate model supported nm catalysts, including wetness impregnation, vacuum vapor deposition, electron-beam lithography, spin-coating, and vesicle-mediated deposition. Recent simulations of the kinetics of heterogeneous reactions occurring on supported catalyst particles are discussed as well. The attention is focused on such effects as reactant supply via the support, interplay of the reaction kinetics on different facets and edges, and adsorbate-induced reshaping of catalyst particles.

Development and Application of Physicochemical Methods for Catalysts Investigation

X-RAY PHOTOELECTRON SPECTROSCOPY OF SUPPORTED METAL CATALYSTS

A.I. Boronin

Condensed Media & Interface Boundaries, 2 (2000) pp. 4-10.

XPS application to highly dispersed catalysts composed of small supported metal particles on the surface of oxides or carbon materials is discussed. The core level chemical shift of the active components of supported catalysts is analyzed with regard to the initial and final states. The role of the metal particle size and the metal support interaction in the energy relaxation process is shown to be important for analysis of photoelectron spectra. The effect of the static charge distribution on the metal and support particles is also considered. Some experimental examples demonstrating complicated nature of the photoionization in the metal-support systems are presented.

HIGH TEMPERATURE DECOMPOSITION OF ETHYLENE AND METHANE AT Pt (111) SURFACE. COMPARATIVE STUDY BY *IN SITU* XPS AND XAES

R.I. Kvon, A.I. Boronin

Condensed Media & Interface Boundaries, 2 (2000) pp. 29-32.

Adsorption of methane and ethylene was studied in the temperature range of 570-970 K by X-Ray

Photoelectron Spectroscopy (XPS) and X-Ray excited Auger Electron Spectroscopy (XAES). Ethylene decomposition at T>770 K leads to the formation of the graphite islands on the surface of Pt (111). It was shown that methane decomposition does not result in the graphite formation but leads to chemisorbed carbon adsorbed layer only. For the methane interaction this temperature range is characterized by the increased diffusion rate of carbon into the Pt bulk, so no carbon aggregation takes place.

XPS STUDY OF CARBON SPECIES AT THE SURFACE OF PLATINUM SINGLE CRYSTAL PLANES

R.I. Kvon, S.V. Koshcheev, A.I. Boronin

J. Molec. Catal. A: Chemical, 158 (2000) pp. 297-300.

Carbonaceous deposits obtained by ethylene decomposition on the surface of (111), (110) and (100) planes of Pt were studied by XPS in the wide temperature range of 570-1470 K. Three different carbon states were found depending on the temperature and Pt plane chosen. At T < 770 K adsorbed state of carbon is formed at all three planes studied. Higher adsorption temperature results in graphite formation at Pt (111) and diamond-like carbon at two other planes.

XPS AND TEM STUDY OF NEW CARBON MATERIAL: N-CONTAINING CATALYTIC FILAMENTOUS CARBON

R.I. Kvon, G.N. Il'initch, A.L. Chuvilin,
V.A. Likholobov

J. Molec. Catal. A: Chemical, 158 (2000) pp. 413-416.

N-containing fibrous carbon material prepared by decomposition of CH_4/H_2/pyridine mixtures over Ni-Cu catalysts has been studied by X-ray Photoelectron Spectroscopy and Transmission Electron Microscopy. The essential effect of the decomposition temperature (in the range of 820-1020 K) and reaction mixture composition on the nitrogen content, its chemical state and the texture of produced carbon filaments was found.

XPS AND SIMS CHARACTERIZATION

V.I. Bukhtiyarov

Catal. Today, 56 (2000) pp. 403-414.

XPS study V_2O_5-WO_3/TiO_2 mixed oxide catalysts for Selective Catalytic Reduction (SCR) of NO_x carried out by researchers from different laboratories shows good reproducibility of the chemical shift results. The binding energies of the corresponding core level spectra allow to identify the chemical states of main elements as Ti(IV), V(V) and W(VI). No other oxidation states for these elements were observed both for fresh/used and for crushed/monolith samples. Discrepancy in quantitative data can be proposed to arise from the heterogeneity of their composition as a function of depth. This suggestion is confirmed by SIMS data and ion etching experiments which indicate surface location of V_2O_5 phase, as well as impurity ones, with respect to TiO_2 and WO_3 and their redistribution as result of catalyst operation.

XPS, TPD AND TPR STUDIES OF Cs-O COMPLEXES ON SILVER: THEIR ROLE IN ETHYLENE EPOXIDATION

E.A. Podgornov, I.P. Prosvirin, V.I. Bukhtiyarov

J. Molec. Catal. A: Chemical, 158 (2000) pp. 337-343.

Various Cs oxides formed on the Ag(111) and Ag(110) single crystals depending on cesium coverage, oxygen pressure have been identified by XPS and TPD. The comparison of the determined characteristics with the data for the Ag/Al_2O_3 catalysts allows to select those of the Cs-O structures which are common for both types of samples: cesium peroxide and cesium suboxide. Mechanisms of their influence onto routes of ethylene oxidation are discussed.

THE COMBINED APPLICATION OF XPS AND TPD TO STUDY OF OXYGEN ADSORPTION ON GRAPHITE-SUPPORTED SILVER CLUSTERS

V.I. Bukhtiyarov, V.V. Kaichev

J. Molec. Catal. A: Chemical, 158 (2000) pp. 167-172.

Oxygen adsorption on supported silver depending on the cluster sizes is studied by XPS and TPD using a model carbon-supported silver catalyst. It has been shown that the electrophilic oxygen active in ethylene epoxidation is produced on the small silver clusters (≤100 Å) more effectively than on the bulk metal, most probably, due to formation of subsurface oxygen. The desorption of the electrophilic oxygen at 450 K proves the thermodynamic possibility of its participation into ethylene oxide formation. Enlargement of the silver particles decreases the amount of subsurface oxygen and result in the appearance of nucleophilic oxygen. These results are used for discussion on the possible explanation of the size effect in ethylene epoxidation over Ag/Al_2O_3 catalyst.

XPS STUDY OF THE SILICA-SUPPORTED Fe-CONTAINING CATALYSTS FOR DEEP OR PARTIAL HYDROGEN SULFIDE OXIDATION

G.A. Bukhtiyarova, V.I. Bukhtiyarov,
N.S. Sakaeva, V.V. Kaichev, B.P. Zolotovskii

J. Molec. Catal. A: Chemical, 158 (2000) pp. 251-255.

Catalytic properties of silica-supported Fe-containing catalysts for deep or partial H_2S oxidation have been correlated with their surface composition characterized by XPS. This allows to show that iron sulfate supported on silica is active in sulfur production with 100% selectivity, whereas the decrease in selectivity to sulfur is accompanied by the appearance of iron disulfide phase in the catalyst. It has been revealed that FeS_2 formed under the reaction conditions is unstable and is easily transformed to sulfate in few days under ambient conditions. This should be taken into account when Fe-containing catalysts for H_2S oxidation are *ex-situ* characterized by physical methods.

NICKEL REINFORCED CATALYSTS OVER A HEAT EXCHANGING SURFACE FOR BENZENE HYDROGENATION

M.M. Danilova, N.A. Kuzin, V.A. Kirillov,
N.A. Rudina, E.M. Moroz

React. Kinet. & Catal. Lett., 69 (2000) pp. 317-324.

X-ray technique, mercury porosimetry and electron microscopy were used to study the regularities of formation of porous metallic nickel-aluminum supports reinforced with a steel grid and distributed over a heat exchanging surface, and of nickel catalysts supported on them. Such catalysts are active in gas phase benzene hydrogenation and also possess high heat conductivity.

ENHANCED REFLECTANCE X-RAY ABSORPTION FINE STRUCTURE SENSITIVITY USING A WHISPERING-GALLERY WAVEGUIDE

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K.V. Zolotarev[b,c]
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Nuclear Instrum. & Methods in Phys. Res. A, 448 (2000) pp. 173-178.

A new technique of reflectance X-ray absorption fine structure (REFL-XAFS) utilizing waveguides where X-rays are reflected many times along the waveguide surface is discussed. The multiple total reflection (MTR) phenomenon highly increases X-ray interaction with the waveguide surface and hence offers higher sensitivity compared to conventional (single reflection) REFL-XAFS. On the one hand, this technique is a direct structural method for characterizing waveguides (e.g. capillaries) where the application of other methods is very difficult. On the other hand, the conventional thin wafer can be transformed to a whispering-gallery (WG) waveguide by bending to a curved mirror. Ray tracing calculations demonstrate that the WG waveguide is very suitable for REFL-XAFS measurements. This method was experimentally realized for a cylindrically bent silica wafer with the surface covered with a GeO_2 monolayer. The Ge K-edge REFL-XAFS measurements were performed using both MTR and conventional techniques. The MTR technique allows to achieve about 20-fold gain in the signal-to-background ratio compared with the conventional technique. The MTR phenomenon discussed can provide new possibilities to study clean surfaces, ultrathin films and adsorbed molecules.

HIGH-QUALITY SYNTHETIC DIAMONDS FOR SR APPLICATION

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A.G. Sokol*, A.F. Khokhryakov*, G.M. Rylov*,
V.A. Chernov, I.N. Kupriyanov** (*Institute of Mineralogy and Petrography, Novosibirsk, Russia; **Institute of Automation and Electrometry, Novosibirsk, Russia)

Nuclear Instrum. & Methods in Phys. Res. A, 448 (2000) pp. 179-183.

Synthetic diamond single crystals grown by the temperature gradient method using BARS technique have been characterized by means of X-ray diffraction. X-ray transmission topography revealed high lattice perfection of the crystals studied. From rocking curves measurements it was found that the width for C(220) reflection varies in the range 5-20 arcsec and depends on the diamond's growth conditions. Application of the diamond crystals as quarter-wave plates for synchrotron X-rays has been tested. The achieved degree of circular polarization is 0.96 at Fe K-edge region. These crystals permit one to apply diamond quarter-wave plates in experiments with divergent and tunable monochromatic beams of bending magnets.

STRUCTURE OF MgO-BASED CATALYSTS MODIFIED WITH $Mg(NO_3)_2$ AND $LiNO_3$

L.M. Plyasova, N.A. Vasilieva, T.A. Krieger,
A.N. Shmakov, G.S. Litvak

Kinetics & Catalysis, 41 (2000) pp. 557-560.

The structure of magnesium oxide prepared by hydration in lithium nitrate and magnesium nitrate solutions and further thermal treatment is examined by X-ray analysis on a precision diffractometer using synchrotron irradiation. Magnesium oxide with a distorted lattice is formed when this preparation procedure is used, and the symmetry is reduced from cubic to rhombohedral. Distortions were more pronounced in the case of a sample treated with magnesium nitrate. The distortions are due to NO_3 groups incorporated into the oxygen framework of the oxide. Such a structure is stable up to 1000 °C. The defects formed lead to the structure and charge inhomogeneity of the crystalline lattice. It is likely that these defects are responsible for the high catalytic activity of the samples.

X-RAY-SENSITIVE STORAGE PHOSPHORS WITH THE OPTICALLY STABLE LUMINESCENT CENTERS

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V.I. Kochubey*, Y.G. Sedova*, D.I. Kochubey,
G.N. Kulipanov, V.V. Lyakh**, V.F. Pindyurin****
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Nuclear Instrum. & Methods in Phys. Res. A, 448 (2000) pp. 196-199.

NaCl, KCl, KBr and LiF crystals doped by In, Tl, Ni, Pd and Ca were investigated as X-ray-sensitive materials. Influence of the way of doping of an impurity and growing of a crystal on such parameters of a material as: sensitivity to ionizing radiation; radiative, optical and thermal stability of the image, obtained after an irradiation is investigated. As a result of the work, media for recording of the X-ray images are developed. These allow to reproduce the images in a mode of a photoluminescence. Spatial resolution and the dynamic range of registration of the developed materials concede to similar parameters of commercial storage luminophores like “Image Plates” based on BaFBr:La. At the same time, as distinct from “Image Plates”, the developed radiophotoluminophores allow a long storage and multiple readout of the information recorded.

SIMULATION OF X-RAY POWDER DIFFRACTION PATTERNS FOR LOW-ORDERED MATERIALS

S.V. Cherepanova, S.V. Tsybulya

J. Molec. Catal. A: Chemical, 158 (2000) pp. 263-266.

A new program for simulation of X-ray diffraction patterns of polycrystalline materials with different kinds of imperfections has been developed. These calculations are performed on the base of the model of one-dimensional (1D) disordered crystal being the statistical sequence of the biperiodic layers. Each layer is characterized by its structure, thickness and probability of occurrence. The sequence of layers is specified with the use of order-disorder parameters and some probability coefficients. Such defects as small sizes of coherently scattering domains (CSD), microstrains and stacking faults are taken into account. Our program simulates two kinds of layers: isotropic (circle) and anisotropic (rectangle). Along with mean sizes of CSD, the variances of normal or lognormal size distributions of CSD can be taken into account. Also, the program makes it possible to specify whether the fluctuations in the layer position are correlated or not. The plane groups of symmetry are introduced to reduce the run time. The background is approximated by using the smoothing spline-functions. The correlation for instrumental line broadening is calculated with a standard. Simulated diffraction pattern is compared and fitted for best correspondence with the experimental one.

Real structures of some specimens have been investigated with this program. These are metastable Ni-In alloys prepared by mechanochemical synthesis, filamentary carbons and metallic Co with microdomain structure.

DIFFRACTION METHOD FOR STRUCTURE INVESTIGATIONS OF SEMICONDUCTOR HETEROSYSTEMS USING SYNCHROTRON VARIABLE WAVELENGTH

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Nuclear Instrum. & Methods in Phys. Res. A, 448 (2000) pp. 282-285.

The synchrotron investigation method is presented for structure research of semiconductor heterosystems with homogeneous layers and superlattices using the variable wavelength of a synchrotron radiation beam passing at the immobile sample. The used experimental procedure is potentially suitable for *in situ* X-ray diffractometry during the growth of epitaxial layers. For the proposed procedure, the equations are derived for the first time to measure tetragonal crystal lattice distortions and superlattice period distribution. The experimental results have been obtained for heterosystems with layers of $Al_xGa_{1-x}As$ grown by molecular-beam epitaxy (MBE) onto GaAs substrates.

HIGH-RESOLUTION X-RAY STUDY OF SPECULAR AND DIFFUSE SCATTERING FROM Ni/C MULTILAYER UPON ANNEALING

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Nuclear Instrum. & Methods in Phys. Res. A, 448 (2000) pp. 276-281.

A high-resolution X-ray diffraction study of specular and diffuse scattering from a Ni/C multilayer upon annealing was performed to examine its optical characteristics and the structural changes of interfacial roughness. The Ni/C multilayer was deposited by the laser ablation technique. The data obtained at the optimal annealing temperature (about 590 K), show a drastic improvement in the reflectivity of the first Bragg order by a factor of 2.4, up to 81%, without any worsening of X-ray optical characteristics and any changes of macroroughness. It supports previous conclusion that annealing at the optimal temperature causes the spinodal decomposition of the interfacial range between the metal and carbon layers. Both the improvement of the sharpness of the boundaries and an increase of the X-ray optical contrast provide a gain in reflectivity.

X-RAY ABSORPTION STUDY OF THE CuO_2 PLANE IN $Nd_{2-X}Ce_XCuO_{4-\delta}$

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Nuclear Instrum. & Methods in Phys. Res. A, 448 (2000) pp. 358-363.

The local structure of the CuO_2 planes in $Nd_{2-x}Ce_xCuO_{4-\delta}$ (x=0, 0.015; δ~0.01) has been examined by temperature-dependent Cu K-edge extended X-ray absorption fine structure (EXAFS) spectroscopy. Three different Cu-O distances can be extracted up to at least 100 K, indicating that the atomic structure of the CuO_2 planes deviates from the *T'* structure much more than it was expected. Positions of the displaced O1 atoms for x=0.15 were obtained from comparative analysis of the experimental and calculated polarized Cu K-edge X-ray absorption near-edge structure, taking into account many-body excitations in the CuO_2 planes.

COMPARISON OF ATOMIC STRUCTURE ANISOTROPY BETWEEN Co-Pd ALLOYS AND Co/Pd MULTILAYER FILMS

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Phys. Rev. B, 62 (2000) pp. 3025-3028.

The Co *K*-edge extended X-ray absorption fine structure measurements with linear polarization dependence have been employed to investigate the chemical short-range order (SRO) and interatomic distance anisotropy in Co_XPd_{1-X} alloy (X = 0.16, 0.31) and $[Co(2\ Å)/Pd(Y\ Å)]_{13}$ multilayer films (Y = 15, 32). The SRO parameters of in-plane first nearest neighbors, 0.063–0.068 in the alloys and 0.012–0.036 in the multilayers, are observed. Surprisingly, these counterintuitive results show clear evidence that the Co atoms at the Co/Pd interfaces in multilayers have more alloylike characteristic than those in alloys with respect to local chemical environment.

MODELING OF THE CURVE RADIAL ELECTRONIC DENSITY DISTRIBUTION FOR AMORPHOUS Me-Zr-O SYSTEMS

E.M. Moroz, A.S. Ivanova, D.A. Zyuzin

J. Molec. Catal. A: Chemical, 158 (2000) pp. 313-317.

Me-Zr-O systems were studied with X-ray Radial Electronic Density Distribution (REDD) method. Data on the known oxides and hydroxides structures, such as interatomic distances (r) and coordination number (Z) were used for the calculated curves. The values r and Z were calculated from the data of structural type, spatial group, coordinates of atom and parameters of cell. For Fe-Zr-O system it has been demonstrated that all samples have similar structures, which related to that of cubic α-ZrO_2. The model with statistical arrangement of Fe^{3+} cations, vacancies in the cation and anion sublattices and modification of anion sublattice with OH^- groups is admitted as most probable. Number of cation and anion vacancies and number of OH^- groups were evaluated using experimental REDD curves of samples.

SURFACE VANADIUM COMPOUNDS IN SUPPORTED VANADIUM-MAGNESIUM CATALYSTS FOR ETHYLENE POLYMERIZATION: X-RAY PHOTOELECTRON AND INFRA-RED DIFFUSION REFLECTANCE SPECTROSCOPY STUDIES

M.A. Mats'ko, I.P. Prosvirin, T.B. Mikenas, V.A. Zakharov, E.A. Paukshtis, V.I. Bukhtiyarov, I.G. Danilova

J. Molec. Catal. A: Chemical, 158 (2000) pp. 443-446.

Adsorption of NO as a probe molecule in infrared diffusion reflectance spectroscopy (DRIFTS) and X-ray photoelectron spectroscopy (XPS) have been used in order to identify surface vanadium species in vanadium-magnesium catalysts (VMC). The presence of V^{3+} and V^{4+} in $VCl_4/MgCl_2$ and V^{4+} in $VOCl_3/MgCl_2$ was shown by XPS and DRIFTS. However, DRIFTS has some limitations due to oxidation of V^{3+} by reaction with NO; moreover, apparently ions V^{5+} and V^{2+} do not absorb NO. The possible identification of surface ions V^{5+} and V^{2+} in VMC using XPS has been demonstrated. Practically in all cases ($VCl_2/MgCl_2$ and $VOCl_3/MgCl_2$) one can see a mixture of vanadium ions in different oxidation and coordination states.

THE APPLICATION OF ADSORBED MOLECULES AS PROBES FOR EXAFS STUDY OF SURFACE

V.V. Kriventsov, D.I. Kochubey

Nuclear Instrum. & Methods in Phys. Res. A, 448 (2000) pp. 308-313.

This work is devoted to some aspects and problems of application of adsorbed molecules as probe for EXAFS study of surface. Two systems were investigated: (1) Ni/C – nickel catalysts of obtaining of carbon by methane decomposition, (2) α-Fe_2O_3 - α-iron oxides prepared in two ways, namely, by oxalate and goethite decomposition. The perspective of the used approach for surface testing of catalysts and for study of reaction courses is shown. However, it is clear from the work that it is necessary to have a wide set of probes, both selectively and non-selectively adsorbed on the surface.

THE DETERMINATION OF ADSORPTION SITE STRUCTURES OF HIGH DISPERSED OXIDES BY EXAFS SPECTROSCOPY USING MOLECULES AS PROBE

V.V. Kriventsov, D.I. Kochubey

J. Molec. Catal. A: Chemical, 158 (2000) pp. 287-291.

The structure of adsorption sites of highly dispersed oxides, such as TiO_2, Fe_2O_3, and ZnO, was investigated by means of H_2Se adsorption. The nanoparticles were studied with a specific surface area not less than 50 m^2/g. The oxide surface was activated either by mechanical activation or by high temperature treatment in a gas flow. Irreversible H_2Se adsorption was carried out up to saturation in H_2 excess at room temperature. EXAFS spectra of the Se-K edge were measured and analyzed. The ratio between point and extended defects as a function of the activation conditions was determined for TiO_2. It was shown that oxygen, being removed from the Fe_2O_3 surface during the activation, is not associated with the presence of a cation in the interstitial position. It was shown for ZnO that a change in the ratio between cation and anion vacations depends on the duration of the mechanical treatment. Perspectives of this approach and possibilities of using the probes are described.

EXAFS AND X-RAY RED STUDY OF POLYMETAL CARBOSYLANES

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Nuclear Instrum. & Methods in Phys. Res. A, 448 (2000) pp. 314-317.

Using EXAES and X-ray RED methods the phase composition of polycarbosylanes containing zirconium has been investigated. It has been demonstrated that metal complex decomposes with introduction into polycarbosilane and formation of metal nanoparticles with the size not exceeding 2 nm and modification of the matrix structure occur. Interaction of the introduced metal with matrix occurs during calcination of sample at 1373-1473 K in nitrogen with forming of zirconium silicide.

EXAFS STUDY OF Cu/C CATALYSTS

V.V. Kriventsov, O.V. Klimov, O.V. Kikhtyanin, K.G. Ione, D.I. Kochubey

Nuclear Instrum. & Methods in Phys. Res. A, 448 (2000) pp. 318-322.

A local arrangement of copper in Cu/C catalysts for dimethylcarbonate synthesis was studied by EXAFS. The samples with various Cu content were prepared by impregnating of carbon carrier “Sibunit” with the alcohol solution of $CuCl_2$. It was determined, that the oxygen atoms from surface groups of carrier always enter into copper surrounding and the relative content of oxygen drops with the increase of Cu content in the samples. The structure of surface copper compounds for initial catalysts was proposed. Thus, samples with low Cu content ($9x10^{-4}$ mol/g-cat) possess surface compounds [carrier-COO-CuCl] or [carrier-CO-CuCl], further, by increasing copper content a second surface layer consisting of hydrated $CuCl_2$ non-bonded with carrier is formed.

A DISTINCTIVE FEATURE IN THE IR SPECTRA OF PROTON DISOLVATES [L_2H^+] AND POLYSOLVATES [(L_2H^+)·nL]: UNUSUAL STRONG BROADENING OF SOME ABSORPTION BANDS OF LIGANDS L BOUND WITH H^+

E.S. Stoyanov

Phys. Chem. Chem. Phys., 2 (2000) pp. 1137-1145.

An IR study of proton disolvates in organic solutions of $L_2H^+{\cdot}FeCl_4^-$, where L = tributyl phosphate (TBP), butyl acetate, diethyl ether, acetone and ethanol, or proton polysolvates of $[(L_2H^+){\cdot}nL{\cdot}FeCl_4^-$ or $(L'H+L)L'{\cdot}FeCl_4^-$ (L = ethanol, L′ =TBP) under the weak polarizing influence of $FeCl_4^-$ anion on the cation led to the discovery of an unusual, very strong broadening of the adsorption bands of the molecular groups of ligands L, which are directly bound with H^+. These bands belong to (i) highly characteristic vibrations of double bonds P=O(-H^+), C=O(-H^+), *etc*., weakly mixed with the vibration of conjugated bonds, and (ii) strongly interacting group vibrations experiencing the influence of the proton. This effect is best exhibited in the IR spectra of proton solvates $H^+{\cdot}nL$ with the positive charge located mainly on one O-H^+-O group. The following explanation of this effect can be proposed. The potential functions of the proton in the O-H^+-O group is almost a single minimum with a flat bottom. Therefore, H^+ is delocalized in a certain spatial interval between the oxygen atoms. As a result, the force constants of the bands of ligands L influenced by H^+ change with the same frequencies as the proton migrates at the bottom of the flat potential minimum. This frequency may be comparable to those of some normal vibrations or exceed them. It has been shown that the same effect also takes place in the IR spectra of proton hydrates $H_5O_2^+{\cdot}nL$, where L = H_2O or organic bases. The effect reported can form a basis for a new interpretation of the peculiarities in the IR spectra of proton hydrates.

UNUSUAL STRONG BROADENING OF SOME ABSORPTION BANDS IN THE IR SPECTRA OF ORGANIC MOLECULES BONDED WITH H^+ IN DISOLVATES [L^-H^+-L]

E.S. Stoyanov

Mendeleev Commun., 5 (1999) pp. 190-191.

An unusual feature has been detected in the IR spectra of the proton disolvates L–H^+–L, namely strong broadening of the absorption bands of molecular groups of the organic ligand L directly bonded with H^+.

INFRARED SPECTROSCOPY TO STUDY THE MECHANISM OF CATALYTIC REACTION ON MOLECULAR SCALE FROM DIFFUSION TO LIMITING STAGE KINETICS

E.A. Paukshtis

J. Molec. Catal. A: Chemical, 158 (2000) pp. 37-44.

Reported here are results recently obtained at the Institute of Catalysis with the IRS of adsorbed molecules used to study the mechanisms of catalytic reactions occurring on the surface of heterogeneous catalysts. It has been found that the structure and strength of OH groups complexes with diffusing molecules (M) are the key factors determining the rate of molecules transfer inside the zeolite crystal. Stoichiometry 2M:1OH appears to provide a higher diffusion rate. Original procedures allowing the identification of surface species nature were designed. One of these procedures is based on a quantitative measurement and dosing at a joint adsorption of reagents and probe molecules. Using a joint adsorption of CO and *tert*-butyl chloride on fluorinated alumina, it has been proved that *tert*-butyl chloride forms complexes with the Lewis sites through the chlorine atoms. The alternating adsorption of aromatic molecules and ammonia proved the aromatic molecule protonation on V_2O_5/Al_2O_3 catalyst. A lot of examples of IR mechanistic studies of catalytic reaction on surface are presented. There are butyl alcohol dehydration, methane partial oxidation, *n*-butyl amine deamination, NO_x selective reduction.

IR-SPECTROSCOPIC INVESTIGATION OF CATION DISTRIBUTION IN Zn-Co OXIDE CATALYSTS WITH SPINEL TYPE STRUCTURE

G.N. Kustova, E.B. Burgina, G.G. Volkova,
T.M. Yurieva, L.M. Plyasova

J. Molec. Catal. A: Chemical, 158 (2000) pp. 293-296.

The structure of Zn-Co spinel prepared by coprecipitation was studied by IR spectroscopy. The characteristic bands of extra OH^- and H_3O^+ groups were shown to exist in IR spectra up to 700^{0}C. After comparing IR spectra of a poorly crystallized low temperature catalyst with that of perfect Zn-Co spinel, the noticeable splittings and shifts of the F_{1u} bands have been associated with definite structural distortions. The presence of extra anions in the catalyst with a spinel-like structure in the temperature region 100-700^{0}C is the factor that stabilized the unusual cation distribution in this catalyst. The most plausible cation distribution in such a spinel is proposed as follows: Co^{3+} and Zn^{2+} are in octahedral positions, and Co^{2+} and Zn^{2+} are in tetrahedral ones.

IN SITU FTIR STUDY OF THE ADSORPTION OF FORMALDEHYDE, FORMIC ACID, AND METHYL FORMATE AT THE SURFACE OF TiO_2 (ANATASE)

G.Ya. Popova, T.V. Andrushkevich,
Yu.A. Chesalov, E.S. Stoyanov

Kinetics & Catalysis, 41 (2000) pp. 805-811.

The catalytic properties of TiO_2 (anatase) in the reactions of formaldehyde oxidation and formic acid decomposition are examined. At 100-150°C, formaldehyde is converted into methyl formate with high selectivity regardless of the presence of oxygen in the reaction mixture. Formic acid is decomposed to CO and water. Surface compounds formed in the reactions of formaldehyde, formic acid, and methyl formate with TiO_2 (anatase) are identified by *in situ* FTIR spectroscopy. In a flow of a formaldehyde-containing mixture at 100°C, H-bonded HCHO, dioxymethylene species, bidentate formate, and coordinatively bonded HCHO are observed on the TiO_2 surface. In the adsorption of formic acid, H-bonded HCOOH and two types of formates (bidentate and unsymmetrical formates) are formed. In the adsorption of methyl formate, H-bonded $HCOOCH_3$, $HCOOCH_3$ coordinatively bonded via the carbonyl oxygen, and bidentate formate are identified.

FTIRS STUDY OF THE NATURE AND REACTIVITY OF THE PRODUCTS OF NITROMETHANE TRANSFORMATION ON THE SURFACE OF COPPER- AND COBALT-EXCHANGED ZSM-5 ZEOLITES AS RELATED TO THE MECHANISM OF NO_X CH_4- SCR

S.A. Beloshapkin, E.A. Paukshtis, V.A. Sadykov

J. Molec. Catal. A: Chemical, 158 (2000) pp. 355-359.

For Cu- and Co-ZSM-5, at temperatures around 300°C, adsorption of nitromethane followed by its acid-catalyzed transformation into isocyanates and melamine as well as reactivity of these species with respect to oxygen and NO were studied by FTIRS. Both species easily interact with molecular oxygen, while no reaction with NO was observed. In the course of melamine oxidation, partial oxidation products including isocyanates appear to be produced. The reactivity of melamine and isocyanate depends upon the temperature and nature of transition metal cation, being reasonably high to suggest their role as intermediates in the NO_x CH_4-SCR.

NATURE OF THE PEROVSKITES SURFACE CENTERS AS STUDIED BY THE INFRARED SPECTROSCOPY OF ADSORBED NO TEST MOLECULE

L.A. Isupova, A.A. Budneva, E.A. Paukshtis,
V.A. Sadykov

J. Molec. Catal. A: Chemical, 158 (2000) pp. 275-280.

FTIRS spectroscopy of adsorbed NO revealed variety of the types of coordinatively unsaturated surface cations for lanthanum cobaltites, manganites and ferrites, some of which emerge due to room-temperature surface reduction by the test molecule. For the surface of $LaFeO_3$, clusters of coordinatively unsaturated Fe^{2+} cations associated with genetic defects dominate. For the surface of $LaCoO_3$ and

$LaMnO_3$ coordinatively unsaturated Me^{+3} cations are mainly revealed being more coordinated by oxygen for the former system. These results could be used to analyze the catalytic properties of perovskites in the reaction of CO oxidation provided density of surface sites and reaction mechanism are taken into account.

MULTINUCLEAR NMR SPECTROSCOPIC CHARACTERIZATION OF VANADIUM(V) ALKYLPEROXO COMPLEXES $VO(OOtBu)_k(OnBu)_{3-k}$, WHERE k=1, 2, 3

D.E. Babushkin, E.P. Talsi

React. Kinet. & Catal. Lett., 71 (2000) pp. 115-120.

Using ^{51}V, ^{17}O, ^{13}C and ^1H NMR spectroscopy, vanadium(V) alkylperoxo complexes $VO(OOtBu)_k(OnBu)_{3-k}$, where k=1, 2, 3, were characterized in the reaction of $VO(OnBu)_3$ with *t*BuOOH in CH_2Cl_2.

MECHANISM OF DIMETHYLZIRCONOCENE ACTIVATION WITH METHYLALUMINOXANE; NMR MONITORING OF INTERMEDIATES AT HIGH Al/Zr RATIOS

D.E. Babushkin, N.V. Semikolenova, V.A. Zakharov, E.P. Talsi

Macromol. Chem. Phys., 20 (2000) pp. 558-567.

Using ^1H and ^{13}C NMR spectroscopy, the interaction between Cp_2ZrMe_2 and MAO in toluene solutions was investigated in the wide range of Al/Zr ratios (10-4000). Several intermediates (**I-IV**) were detected in the reaction. The structures of these intermediates were elucidated from detailed analysis of ^{13}C-^1H NMR data. Intermediate I is a weak complex of Cp_2ZrMe_2 with the Lewis acidic sites of MAO: $Cp_2MeZr\text{-}Me\rightarrow Al\equiv(I)$. Free Cp_2ZrMe_2 is in the fast in the NMR time-scale exchange with **I**. Intermediate **II** is the complex contact ion-pair $[Cp_2ZrMe(\mu\text{-}Me)Cp_2ZrMe]^+[Me\text{-}MAO]^-$ having symmetric binuclear cationic part. Species IIIa↔IIIb are heterodinuclear complex $[Cp_2ZrMe(\mu\text{-}Me)_2AlMe_2]^+[Me\text{-}MAO]^-$ contact ion-pairs and similar separated ion-pairs. Species **IV** can be represented by unsymmetrically Me-bridged complex $Cp_2MeZr^+\leftarrow Me^-\text{-}Al\equiv(MAO)$. Reaction equilibria involving intermediates **I-IV** were studied varying Al/Zr ratio, MAO concentration, Al_2Me_6 content, and temperature. On increasing of Al/Zr ratio, complexes **I, II** and free Cp_2ZrMe_2 gradually disappear and at high Al/Zr ratios in conditions, close to the usual polymerization conditions, only species **III** were detected. At constant Al_2Me_6 the concentration of **III** but not of **IV** correlates with available data on polymerization activity as a function of Al/Zr ratio. The possible scheme of Cp_2ZrMe_2 interaction with MAO and catalytically active cationic species $[Cp_2ZrMe]^+$ formation is suggested. Data on Cp_2ZrCl_2 and MAO are given for comparison.

SODIUM-MODIFIED V_2O_5-TiO_2 CATALYSTS: ^{23}Na AND ^{51}V SOLID-STATE NMR STUDY

V.V. Terskikh, O.B. Lapina, V.M. Bondareva

Phys. Chem. Chem. Phys., 2 (2000) pp. 2441-2448.

Sodium-doped binary vanadia-titania catalysts were studied using modern high-resolution solid-state NMR techniques, including fast magic angle spinning (MAS) and two-dimensional triple-quantum MAS NMR. The latter technique was engaged in the interpretation of second-order quadrupolar broadened one-dimensional ^{23}Na MAS NMR spectra. NMR and X-ray powder diffraction data brought together allow identification of sodium- and vanadium-containing species formed in the course of the preparation of the catalysts. The effect of the sodium concentration on the nature of the resulting species is discussed.

CHARACTERIZATION BY SOLID STATE ^{51}V NMR SPECTROSCOPY

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Catal. Today, 56 (2000) pp. 379-387.

The fresh catalyst V_2O_5-WO_3/TiO_2 and catalyst used in SCR for 9000 h have been studied by the solid state ^{51}V NMR spectroscopy in static and MAS conditions. According to ^{51}V NMR in both samples the majority of vanadium sites are in a distorted octahedral environment similar to that in V_2O_5. There is a strong interaction between vanadium oxide and the support, but the concentration of vanadium atoms strongly bound to the surface is very small and can be detected only in MAS NMR experiments or after removing the excess of V_2O_5. There is no influence of WO_3 additives on the structure of the particles of V_2O_5, whereas the influence on the structure of strongly bounded V cannot be excluded. Combination of static (wide line) and MAS NMR techniques permit the characterization of not only the structure of the vanadium species but also small changes in their local environment. Hence these experiments show that there are some distortions of the local environment of vanadium sites of the vanadium oxide particles compared with the polycrystalline V_2O_5; treatment by SCR increases these distortions.

^{27}Al MAS NMR STUDY OF THE INTERACTION OF SUPPORTED ZIEGLER-NATTA CATALYSTS WITH ORGANOALUMINIUM Co-CATALYST IN THE PRESENCE OF DONOR

A.G. Potapov, V.V. Terskikh, G.D. Bukatov, V.A. Zakharov

J. Molec. Catal. A: Chemical, 158 (2000) pp. 457-460.

^{27}Al MAS NMR spectroscopy has been used to study the surface aluminium compounds formed upon interaction of the supported $TiCl_4$/donor/$MgCl_2$ catalyst with $AlEt_3$ in the presence or absence of the external donor. Similarly with the catalyst without any donors, the $AlEt_2Cl$ formed adsorbs on the catalyst surface. It was found that there is no influence of internal and/or external donors on the state of aluminium in adsorbed $AlEt_2Cl$ in spite of a decrease of the aluminium content in the presence of external donor.

AN ^{1}H NMR MICROIMAGING STUDY OF WATER VAPOR SORPTION BY INDIVIDUAL POROUS PELLETS

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J. Phys. Chem. B, 104 (2000) pp. 1695-1700.

The ^{1}H NMR microimaging technique is applied to study water vapor sorption by the individual cylindrical silica gel and alumina pellets impregnated with hygroscopic salts. The two-dimensional images or the one-dimensional profiles of the sorbed water distribution are detected sequentially to monitor the transport of water within the pellets in real time in the course of the sorption process. The results identify the propagation of the sorbed water front through the dry regions of the pellets as the rate limiting stage of the sorption process. This propagation can be facilitated by employing the pellets with the eggshell distribution of the salt, but in such cases the salt redistributes readily in the course of the sorption process, as revealed by the relaxation weighted ^{1}H NMR microimaging experiments in which paramagnetic salts are used. The diffusion equation with water content dependent diffusivity is employed to model the one-dimensional radial profiles of water distribution within the pellet with appropriate correction for the relaxation weighting effects.

A QUANTITATIVE NMR IMAGING STUDY OF MASS TRANSPORT IN POROUS SOLIDS DURING DRYING

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Chem. Engin. Sci., 55 (2000) pp. 1559-1571.

The temporal transformations of the radial distribution of a liquid in a presoaked porous cylindrical catalyst support pellet detected by ^{1}H NMR microimaging technique in the course of the pellet drying are analyzed quantitatively in terms of the diffusion equation. The approach is shown to be adequate for evaluating the diffusivity and its dependence on the degree of pellet saturation with a liquid, provided that the NMR microimaging data are properly corrected for the relaxation weighting effects. It is demonstrated that for liquids characterized by a low surface tension, such as acetone, benzene and cyclohexane, transformations of the concentration profiles can be adequately modeled assuming a liquid content-independent diffusivity. In contrast, the diffusivity of water in titania and alumina pellets substantially decreases with the decrease of water content. For alumina pellets with a pronounced "bimodality" in the pore size distribution the water concentration dependence of diffusivity is shown to be non-monotonic. It is argued that for liquids with high surface tension, the shape of the concentration profiles and the behavior of diffusivity as a function of liquid content are both related to the shape of the cumulative pore size distribution of the porous solid under study due to the existence of efficient capillary flows induced by capillary suction.

STUDY OF POLARIZED XANES TaL_3 SPECTRA OF 1T-TaS_2 MONOCRYSTALS

T.K. Kim, V.P. Babenko, D.I. Kochubey

Nuclear Instrum. & Methods in Phys. Res. A, 448 (2000) pp. 327-331.

New results concerning the change in polarized XANES spectra and the white line for vertical rotation of 1T-TaS_2 monocrystal were obtained. This change results from the presence of charge density wave superstructure in 1T-TaS_2.

FIRST *IN SITU* ^{1}H NMR SPECTROSCOPIC MONITORING OF MANGANESE SPECIES IN THE Mn^{III}(SALEN) + PhIO CATALYTIC SYSTEM

K.P. Bryliakov, D.E. Babushkin, E.P. Talsi

Mendeleev Commun., 10 (2000) pp. 1-3.

High-valence manganese species formed in the Mn^{III}(salen) + PhIO catalytic system were characterized using ^{1}H NMR spectroscopy.

^{1}H NMR AND EPR SPECTROSCOPIC MONITORING OF THE REACTIVE INTERMEDIATES OF (SALEN)Mn^{III} CATALYZED OLEFIN EPOXIDATION

K.P. Bryliakov, D.E. Babushkin, E.P. Talsi

J. Molec. Catal. A: Chemical, 158 (2000) pp. 19-35.

Using ^{1}H NMR and EPR spectroscopy, manganese species formed in the catalytic systems **1**+iodosobenzene (PhIO) and **1**+meta-chloroperoxybenzoic acid (*m*-CPBA), where 1 is (*R,R*)-(-)-*N,N'*-bis(3,5-di-*tert*-butylsalicylidene)-1,2-cyclohexanediamino-manganese(III) chloride ([Salen)Mn^{III}]) were studied. Three types of manganese complexes were characterized in the catalytic system **1**+PhIO **(4-6).** Complex **4** is very unstable and reacts with styrene at –20°C to afford styrene oxide. It exhibits three signals of *t*Bu groups at 1.68, 1.64 and 1.42 ppm. This pattern closely resembles that for a model complex [(Salen)Mn^V≡N]. Based on these data, **4** was identified as d^2 low-spin oxomanganese(V) complex [(Salen)MnV=O]$^+$. Complexes **5** and **6** are relatively stable at –20°C and poorly reactive towards styrene at this temperature. They display ^{1}H NMR spectra characteristic for antiferromagnetically coupled μ-oxo-dinuclear Mn^{IV} species and are identified as dinuclear complexes [(Salen)LMn^{IV}-*O*-Mn^{IV}(Salen)L'] with L, L'=Cl$^-$ and PhIO. It was found by EPR that the acylperoxo complex (Salen)Mn^{III}(OOCOAr) (**7**) was formed at the first stage of the interaction of **1** with *m*-CPBA in CH_2Cl_2. Complex **7** is unstable and converts into manganese(IV) oxo complex [(Salen)Mn^{IV}(O)] (**8**). The evaluated first order rate constant of this conversion is 0.25±0.08 min^{-1} at –70°C. Complex **7** reacts with styrene with the rate constant 1.1±0.4 M^{-1} min^{-1} at –70°C to give epoxide and restore **1**. Complex **8** is inert towards styrene at low temperature. The effect of donor ligand *N*-methylmorpholine-*N*-oxide (NMO) on the epoxidation of styrene by the system **1**+*m*-CPBA was studied. Addition of NMO (2-5 equiv.) to the solution of **1** in CH_2Cl_2 before interaction with *m*-CPBA was found to dramatically increase the rate of undesirable transformation of the reactive acylperoxo complex **7**-NMO into relatively inert oxo complex **8**-NMO. However, in the presence of styrene, such undesirable conversion is entirely suppressed by very rapid reaction of **8**-NMO with styrene to afford styrene oxide and restore **1**-NMO.

EPR DETECTION AND CHARACTERIZATION OF HIGH-VALENCE MANGANESE COMPLEXES IN Mn^{III}(SALEN) CATALYZED AEROBIC OLEFIN EPOXIDATION

K.P. Bryliakov, I.V. Khavrutskii, E.P. Talsi, O.A. Kholdeeva

React. Kinet. & Catal. Lett., 71 (2000) pp. 183-192.

Intermediates formed in (Salen)Mn^{III}Cl/IBA/O_2 catalytic system and (Salen)Mn^{III}Cl/perisobutyric acid (PIBA) stoichiometric system as well as the effect of the axial ligand, *N*-methylimidasol (*N*-Me-Imd), on these intermediates were first studied using EPR. The interaction of (Salen)Mn^{III}Cl with IBA in the presence of O_2 leads to the formation of L(Salen)Mn^{IV}=O complexes (L=Cl$^-$ and anion of isobutyric acid). The same L(Salen)Mn^{IV}=O species can be obtained by treatment of (Salen)Mn^{III}Cl with stoichiometric amount of PIBA in toluene. The oxo-species L(Salen)Mn^{IV}=O are not able to epoxidize alkenes and form most probably via homolytic cleavage of O-O-bond in active (Salen)Mn^{III}(OOCOR) acylperoxo complex, which is not detectable because of its high reactivity. In the presence of *N*-Me-Imd, a new complex, most likely (Salen)Mn^{IV}(OOCOR)*N*-Me-Imd acylperoxo complex was detected along with mixed-valence dimeric complexes [(Salen)Mn^{III}-(μ_2-O)$_2$-Mn^{IV}(Salen)]. Arguments in favor of two different active intermediates, leading to different epoxide enantiomers in Mukaiyama's system in the presence and in the absence of *N*-Me-Imd, have been found and mechanisms of the formation of these intermediates have been proposed.

KINETICS OF POLYPROPYLENE MACRORADICALS TERMINATION IN THE COURSE OF ITS MODIFICATION

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Polymer Sci., *Ser. B,* 42 (2000) pp. 309-313.

The kinetics of PP macroradicals termination generated under ν-irradiation in the presence of low-molecular-mass compounds immobilized in the polymer matrix, which are used as monomers in free-radical polymerization both active, such as styrene and methyl methacrylate, and inactive, such as vinyltriethoxysilane, was studied by EPR spectroscopy. It was shown that the type of the monomer additives determines the mechanism and the rate of PP macroradicals termination. The effective rate constants for the macroradicals termination in the presence and absence of the low-molecular-mass compounds under examination were calculated.

EPR SPECTROSCOPIC CHARACTERIZATION OF DeNO$_x$ AND SO$_2$ OXIDATION CATALYSTS AND MODEL SYSTEMS

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(*Technical University of Denmark, Lyngby, Denmark)

Catal. Today, 54 (1999) pp. 465-472.

The industrial SO_2 oxidation catalyst VK69 deactivates at around 440°C in a 10% SO_2, 11% O_2, 79% N_2 gas mixture. *In situ* EPR measurements show that the deactivation is caused by precipitation of V(IV) compounds. DeNO$_x$ catalysts based on V_2O_5/TiO_2, the TiO_2 support, analytical grade anatase and transition metal-exchanged Al-PILCs (pillared clay) have been characterized by EPR spectroscopy and the catalytic activity of the catalyst monitored up to 500°C. Depending on the exchanged metal ion, a relatively large temperature range for the catalytic activity towards the SCR reaction was observed.

ON THE DAPS CAPABILITY FOR TESTING THE CHEMISORBED SPECIES LOCATION

A.R. Cholach, V.M. Tapilin

React. Kinet. & Catal. Lett., 71 (2000) pp. 65-70.

The DAPS is used to testify the location of the chemisorbed species resulted from H_2, O_2, NO adsorption and interaction on the Pt(100)-(1x1) single crystal surface. The data obtained evidence that platinum atoms of the first surface layer are influenced in the course of O_2 adsorption, H_2+O_{ads} interaction and NO+H_{ads} interaction. Indeed, due to steric reasons all the possible surface species resulted from these processes must interact with the first platinum layer only. In contrast to that the H_2 adsorption at low exposure mainly affects the platinum atoms of the second layer as it was mentioned above. Therefore, the obtained results testify to high sensitivity of the DAPS technique to the location of surface species relative the top surface layers of Pt(100)-(1x1) single crystal surface.

ELECTRONIC PROPERTIES OF Pt(100) SINGLE CRYSTAL SURFACE: EXPERIMENTAL STUDY AND THEORETICAL CALCULATIONS

A.R. Cholach, V.M. Tapilin

J. Molec. Catal. A: Chemical, 158 (2000) pp. 181-187.

The density of vacant states of Pt(100)-(1x1) single crystal surface is investigated by means of disappearance potential spectroscopy. Probing hydrogen adsorption is used in order to suppress the strong diffraction background and to display the desirable features in difference spectra. Local density of states is calculated for the several top layers of semi-infinite Pt(100)-(1x1) plane. The spectra features are in a good agreement with the peculiarities of electronic structure that resulted from calculations. The comparison of experimental and theoretical data shows that hydrogen atoms adsorbed on the Pt(100)-(1x1) surface at 300 K primarily interact with platinum atoms of the second layer.

FRAGMENTATION OF SiO$_2$ AEROGELS IN AQUEOUS NaOH SOLUTIONS STUDIED *IN SITU* BY SAXS USING SR

A.G. Okunev, A.N. Shmakov, A.F. Danilyuk, Yu.I. Aristov

Nuclear Instrum. & Methods in Phys. Res. A, 448 (2000) pp. 261-266.

Structural deformations of three types of silica aerogels due to their dissolution in aqueous solution of NaOH at pH = 13.6÷13.9 have been explicitly studied *in situ* using small angle X-ray scattering of synchrotron radiation. For all aerogels studied the scattered intensity *I* is found to increase rapidly in the scattering vector range $h = 0.15 \div 0.6$ nm^{-1} that indicates the aerogel threshold disintegration. When the scattering at $h = 0.15$ nm^{-1} reaches the maximum the dependency of Ln*I* on Ln*h* gives a straight line with the slope critically depending on the pH of solution and, to a lesser extent, on the nature of the aerogel. The observed phenomena are discussed in terms of the percolation theory.

A STUDY OF INTERACTION OF VANADIUM TETRACHLORIDE AND VANADIUM OXYTRICHLORIDE WITH ALCOHOLS AND ALUMINUM ALKOXIDE CHLORIDES

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Russ. J. Inorg. Chem., 44 (2000) pp. 521-526.

The interaction of vanadium compounds (VCl_4 and $VOCl_3$) with alcohols (*tert*-butanol and 2-ethyl-1-hexanol) and aluminum alkoxides $Al(OR)_2Cl$ is studied by EPR, ^{51}V NMR, and electronic absorption spectroscopy. ^{51}V NMR evidence shows that the reaction of $VOCl_3$ with alcohols results in a successive substitution of alkoxy groups for the chlorine atoms in vanadium oxytrichloride. In this process, the amount of alcohol required for obtaining di- and trisubstituted alkoxo derivatives exceeds the stoichiometric amounts. Synthesis of alkoxy derivatives of $VOCl_3$ is shown to be accompanied by a side reaction of the reduction of vanadium to V^{4+}. It is found that the reaction of $VOCl_3$ with $Al(OR)_2Cl$ leads to the formation of monoalkoxide derivatives of vanadium oxytrichloride. Upon interaction of VCl_4 with alcohols (*tert*-butanol and 2-ethyl-1-hexanol) or aluminum alkoxides, only two chlorine atoms are replaced by alkoxy groups to form vanadium alkoxide of the composition $V(OR)_2Cl_2{\cdot}ROH$.

MÖSSBAUER SPECTROSCOPY STUDY OF THE ALUMINA-SUPPORTED IRON-CONTAINING CATALYSTS FOR HYDROGEN SULFIDE OXIDATION

N.S. Sakaeva, V.A. Varnek, G.A. Bykhtiyarova,
V.F. Anufrienko, E.A. Sobolev, B.P. Zolotovskii

React. Kinet. & Catal. Lett., 70 (2000) pp. 169-176.

This paper presents the results of the investigation by Mössbauer spectroscopy of the iron state transformation on the $FeSO_4$-impregnated alumina surface depending on pretreatment conditions and the catalytic activity of the samples produced in the H_2S oxidation reaction. The activation of the $FeSO_4$-impregnated Al_2O_3 sample in air flow at 500°C leads to the Fe_2O_3 formation, while pretreatment of the same sample in helium flow containing 2 vol. % of H_2S and 30 vol. % of water vapor at 300°C gives FeS_2. The correlation of these data with the catalytic properties of the corresponding samples allows us to suggest that iron oxide catalyze the hydrogen sulfide oxidation to sulfur, whereas H_2S conversion to SO_2 is governed by FeS_2.

ROLE OF DEFECT STRUCTURE IN STRUCTURAL SENSITIVITY OF THE OXIDATION REACTIONS CATALYZED BY DISPERSED TRANSITION METAL OXIDES

V.A. Sadykov, S.F. Tikhov, S.V. Tsybulya,
G.N. Kryukova, S.A. Veniaminov,
V.N. Kolomiichuk, N.N. Bulgakov, E.A. Paukshtis,
V.P. Ivanov, S.V. Koshcheev, V.I. Zaikovskii,
L.A. Isupova, E.B. Burgina

J. Molec. Catal. A: Chemical, 158 (2000) pp. 361-365.

For dispersed transition metal oxides, specific catalytic activity in the reactions of CO and hydrocarbons oxidation was compared with densities of bulk and surface defects estimated using a combination of diffraction and spectroscopic methods. On this bases, the oxide systems were classified with respect to the scale and origin of the structural sensitivity manifestation. The results were discussed from the point of view of the atomic structure of the most developed surface faces of these oxides and their stoichiometry ranges. The most active surface sites were found to be associated with the surface extended defects including those located at outlets of bulk extended defects.

ORIGIN OF THREEFOLD PERIODICITY IN HIGH-RESOLUTION TRANSMISSION ELECTRON MICROSCOPY IMAGES OF THIN FILM CUBIC SiC

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Microsc. Microanal., 5 (1999) pp. 420-427.

High-resolution transmission electron microscopy (HRTEM) images of the [1-10] zone of cubic SiC layers grown by molecular beam epitaxy (MBE) often reveal regions of material exhibiting an unusual threefold periodicity. In this report it is demonstrated by HRTEM image simulations that the model of the 9R polytype and an alternative twinning model can fit qualitatively the experimental HRTEM images. However, by comparing the fast Fourier transform patterns of the experiments and the simulations, as well as by using dark-field imaging, it has been shown unambiguously that only the model of overlapping twinned 3C-SiC crystals fully agrees with the experiments.

VACANCY ORDERING IN THE STRUCTURE OF γ-Al_2O_3

G.N. Kryukova, D.O. Klenov, A.S. Ivanova, S.V. Tsybulya

J. Europ. Ceram. Society, 20 (2000) pp. 1187-1189.

Defect structure of γ-Al_2O_3 prepared by the thermal decomposition of well-crystallized, high purity boehmite (γ-AlOOH) has been studied by HREM. It was shown that the intrinsic feature of γ-alumina structure is a presence of almost hexagonal closed loops formed due to the ordering of cation vacancies over octahedral positions on (110) and (111) planes. These defects are relatively stable; they are preserved, though being changed in shape, in the γ-alumina sample upon its further calcination until the appearance of traces of δ-alumina phase.

HREM STUDY OF THE NANOSTRUCTURED MOLYBDENUM AND VANADIUM DOPED TITANIA CATALYST

G.N. Kryukova, G.A. Zenkovets, V.N. Parmon

React. Kinet. & Catal. Lett., 71 (2000) pp. 173-176.

$MoO_3/V_2O_5/TiO_2$ (anatase) catalyst with 5 and 20 wt.% loadings of MoO_3 and V_2O_5 has been studied, using high resolution electron microscopy. Main structural peculiarity of this system was found to be the presence of nanometer size layers of a complex Mo-V-O phase on the surface of the titania support. The observed structure seems to be a metastable and may exist only on the surface of TiO_2 particles.

SUPER-ALFVÉN EXPANSION OF A NOVA SHELL IN THE MAGNETIC FIELD OF ITS CORE

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Astronomy Lett., 26 (2000) pp. 362-371.

The effect of nova magnetodipole fields on the dynamics and structure of ejected shells by using a numerical model based on the kinetic–hydrodynamic description of plasma dynamics has been studied. The calculations show that characteristic nonuniformities appear in the distribution of field and plasma perturbations during super-Alfvén shell expansion in the circumstellar medium.

PLATINUM ELECTRODEPOSITS ON GLASSY CARBON: THE FORMATION MECHANISM, MORPHOLOGY, AND ADSORPTION PROPERTIES

O.V. Sherstyuk, S.N. Pron'kin*, A.L. Chuvilin, A.N. Salanov, E.R. Savinova, G.A. Tsirlina*, O.A. Petrii* (*Moscow Lomonosov State University, Moscow, Russia)

Russ. J. Electrochem., 36 (2000) pp. 741-745.

The deposition of platinum on glassy carbon (GC) is studied by chronoamperometry. Basic tendencies of the formation of aggregate platinum particles on the oxidized carbon surface are established. These include a primary instantaneous nucleation of platinum under diffusion control and the beginning of a secondary nucleation prior to filling primary active centers. The deposit morphology is examined by *ex situ* methods of scanning electron microscopy (SEM), transmission electron microscopy (TEM), and scanning tunneling microscopy (STM). A globular structure of platinum, formed by crystallites 3–5 nm in size, is revealed. A comparison of the STM, SEM, and TEM data demonstrates a high information value and accuracy of STM in studies of disperse materials in both nanometer and submicron ranges. Various coulometry techniques intended for the determination of the true surface area of deposited platinum are compared. The most informative techniques are the voltammetry of desorption of copper adatoms and chemisorbed carbon monoxide at, respectively, low and high platinum contents. Differences in the formation kinetics and properties of aggregate particles in Pt/GC and Pt/Pt are found, specifically, smaller Pt/GC crystallites and higher degrees of their concrescence (screening).

THE DETERMINATION OF PROTON AFFINITY FOR OXYGEN-CONTAINING MOLYBDENUM CLUSTERS BY THE METHOD OF ION CYCLOTRON RESONANCE

V.B. Goncharov, E.F. Fialko

Russ. J. Phys. Chem., 74 (2000) pp. 791-793.

Several oxygen-containing molybdenum clusters Mo_xO_y (x=1-3, y=1-9) were prepared in a Knudsen cell combined with an ion trap. The reactions of the clusters with C_1-C_4 protonated alcohols and the ammonium ion were studied by ion cyclotron resonance. The upper and lower proton affinity limits determined for the neutral oxygen-containing molybdenum clusters equaled $PA(MoO)<180$, $PA(Mo_2O_4, Mo_2O_5, Mo_3O_8)=188\pm8$, $PA(MoO_2) = 202\pm5$, and $PA(MoO_3, Mo_2O_6, Mo_3O_9) > 207$ kcal/mol.

INVESTIGATION OF THE STRUCTURE OF PROTOHEMATITE-ACTIVE METASTABLE PHASE OF FERRUM (III) OXIDE

E.B. Burgina, G.N. Kustova, L.A. Isupova,
S.V. Tsybulya, G.N. Kryukova, V.A. Sadykov

J. Molec. Catal. A: Chemical, 158 (2000) pp. 257-261.

A new modification of Fe(III) oxide – protohematite – was produced by thermal decomposition of crystalline hydroxides and salts and by plasma chemical method. Protohematite is a metastable phase which transforms into α-Fe_2O_3 at 1100°C, under pressure or mechanic chemical activation. IR and Raman spectroscopy, X-ray powder diffraction, and transmission electron microscopy were used to study the structure of protohematite. It was concluded that protohematite has unique structural characteristics. The hypothesis concerning the structure of protohematite was suggested. Specific chemical activity of the protohematite was assumed to originate from the presence of some ferric cations in quasi tetrahedral (distorted octahedral) coordination.

PHYSICOCHEMICAL AND CATALYTIC PROPERTIES OF GLASS CRYSTAL CATALYSTS FOR THE OXIDATION OF METHANE

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A.M. Kovalev*, O.A. Bajukov*, N.N. Anshits*,**
E.V. Sokol**, D.I. Kochubey, A.I. Boronin,**
A.N. Salanov, S.V. Koshcheev (*Institute of Chemistry and Chemical Technology, Krasnoyarsk, Russia; **Krasnoyarsk State Technical University, Krasnoyarsk, Russia; ***Institute of Physics, Krasnoyarsk, Russia; ****Institute of Geology, Geophysics and Mineralogy, Novosibirsk, Russia)

J. Molec. Catal. A: Chemical, 158 (2000) pp. 209-214.

Magnetic microspheres and cenospheres recovered from fuel ashes were studied by SEM, XRD, electron probe microanalysis, chemical analysis and Mössbauer spectroscopy. The magnetic microspheres were shown to consist of a crystal phase based on a solid solution of Fe_3O_4-Mg, Mn, Ca-ferrite, α-Fe_2O_3 and a glass phase composed of a calcium ferrite, fayalite, wollastonite, ferrous olivines and mullite. The morphology of globules and size of crystallites of active phase were established to depend on the basicity of the glass phase. It was shown that catalytic activity of magnetic phase were established to depend on the basicity of the glass phase. It was shown that catalytic activity of magnetic microspheres and cenospheres in oxidative conversion of methane is determined by component containing iron and depends on its accessibility and distribution on the surface.

PECULIARITIES OF THE STRUCTURE OF METASTABLE PHASE OF FERRUM (III) OXIDE

E.B. Burgina, G.N. Kustova, S.V. Tsybulya,
G.N. Kryukova, G.S. Litvak, L.A. Isupova,
V.A. Sadykov

J. Struct. Chem, 41 (2000) pp. 489-497.

The results of structure investigations of metastable modification of ferrum oxide, obtained by goethite incomplete dehydration are reported.

STOICHIOGRAPHY AS APPLIED TO STUDYING COMPOSITION AND REAL STRUCTURE OF CATALYSTS

V.V. Malakhov

J. Molec. Catal. A: Chemical, 158 (2000) 143-148.

The general principles of a new concept of chemical analysis, called stoichiography, are presented. Stoichiography allows the reference-free analyzing of the molecular and phase composition of complex substances. The differential dissolving technique as a new stoichiography method was developed to characterize in detail the phase composition of heterogeneous catalysts and to identify known and absolutely unknown phases composing the catalyst. The analyzed phases may be in crystalline or amorphous state, which is of no importance for the analysis performance. Such phase analysis is performed with a high sensitivity and very fast. Equipment, developed specially for this analysis, is called stoichiograph. The advantages of differential dissolving in studying the phase composition of catalysts are demonstrated through many particular examples.

SHTCIES-SELECTIVE ANALYSIS BY MICROCOLUMN MULTICAPILLARY GAS CHROMATOGRAPHY WITH INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRIC DETECTION

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Analytical Chemistry, 71 (1999) pp. 4534-4543.

A glass rod (5-20 cm long, 2 mm o.d.) containing more than 1200 parallel microchannels (36-40 microns i.d.) was converted into a high-resolution (more than 100 theor. plates cm^{-1}) GC column by coating the inside of channel in a way that is compensated for the dispersion of the channel inner diameter. The columns were evaluated for the separation in mixtures of several organometallic (Hg, Sn, Pb) compounds prior to on-line sensitive metal-selective detection by ICP-MS. Chromatographic separation conditions were optimized to enable a rapid (within a maximum 30 sec.) multielemental speciation analysis. Absolute detection limits were 0.1 pg for Hg, 0.05 pg for Sn and 0.03 pg for Pb using the carrier gas flows of about 200 mL min^{-1}. The microcolumn multicapillary GC/ICPMS developed was applied to the analysis of a number of environmental samples. The results were validated with certified reference materials for tin (BCR477, PACS-2) and mercury (DORM-1, TORT-1).

STRUCTURAL STUDY OF X-RAY AMORPHOUS Fe-Zr-O MATERIALS

D.A. Zyuzin, E.M. Moroz, A.S. Ivanova, V.I. Zaikovskii

Inorg. Mater., 36 (2000) pp. 359-363.

Radial-distribution-function analysis was used to study the structure of X-ray amorphous Fe–Zr–O materials prepared by heat treatment between 383 and 673 K. The chemical and structural formulas of the materials were established. The results demonstrate that the introduction of Fe^{3+} into ZrO_2 favors the formation of vacancies and reduces interatomic distances in comparison with cubic ZrO_2. The materials contain OH^- groups, whose concentration decreases with increasing heat-treatment temperature.

RADIOPHOTOLUMINESCENCE OF ALKALI-HALIDE CRYSTALS STIMULATED BY BESSEL LASER BEAM

V.V. Lyakh*, V.F. Pindyurin*, D.I. Kochubey, K.E. Gyunzburg, N.P. Zvezdova**, V.I. Kochubey**, Y.G. Sedova**, V.P. Koronkevich***, A.G. Poleschuk***, A.G. Sedukhin***** (*Budker Institute of Nuclear Physics, Novosibirsk, Russia; **Institute of Mechanics and Physics at Saratov State University, Saratov, Russia; ***Institute of Automation and Electrometry, Novosibirsk, Russia)

Nuclear Instrum. & Methods in Phys. Res. A, 448 (2000) pp. 200-206.

A new approach to realization of optimal high-resolution reading of deep X-ray images in X-ray-sensitive materials on the base of alkali-halide crystals modified with admixtures has been suggested and investigated experimentally. A possibility to use diffraction axicons with ring aperture for forming micron bright light beams (spatially truncated Bessel beams) which can efficiently de-excite radiophotoluminescence centers lying at large depth in crystals is also presented.

ADSORPTION STUDY OF MICROPORE STRUCTURE OF TIN DIOXIDE

V.Yu. Gavrilov

Kinetics & Catalysis, 41 (2000) pp. 276-281.

The micropore structure of xerogels of tin dioxide prepared by precipitation is studied by the physical adsorption of N_2, O_2, and H_2 at –195.6°C. The parameters of the microstructure as a whole depend on the adsorbate. The specific surface area of supermicropores measured by the oxygen adsorption exceeds that measured by nitrogen adsorption, and the extent of excess increases linearly with an increase in the supermicropore volume. The samples of tin dioxides have molecular-sieve properties, but they do not contain ultramicropores measurable by the adsorption of molecular hydrogen.

Nature, Mechanism and Physicochemical Essence of the Low-Waste, Environmentally Friendly Methods of Catalyst Preparation

MECHANOCHEMISTRY OF CATALYSTS

V.V. Molchanov, R.A. Buyanov

Russ. Chem. Rev., 69 (2000) pp. 435-450.

Data on the use of mechanochemical activation for the preparation of catalysts and supports are generalised. The effect of mechanochemical activation on the catalytic properties of various systems is noted. Catalytic reactions occurring under conditions of mechanochemical activation are discussed. The hypotheses concerning the nature of the effect of mechanochemical activation on the reactivity (including catalytic properties) are considered. The bibliography includes 197 references.

POROUS Al_2O_3/Al METAL CERAMICS PREPARED BY THE OXIDATION OF ALUMINUM POWDER UNDER HYDROTHERMAL CONDITIONS FOLLOWED BY THERMAL DEHYDRATION. I. COMPOSITION AND MACROCHARACTERISTICS OF COMPOSITES

S.F. Tikhov, V.B. Fenelonov, V.A. Sadykov, Yu.V. Potapova, A.N. Salanov

Kinetics & Catalysis, 41 (2000) pp. 826-834.

The macrotexture and mechanical properties of porous Al_2O_3/Al metal ceramics prepared by the hydrothermal treatment of aluminum powder in a closed space are studied using gravimetry, pycnometry, mercury porosimetry, and scanning electron microscopy. Analytical expressions that relate the porosity, density, and mechanical strength of parent materials and final products to the composite synthesis conditions are derived.

POROUS Al_2O_3/Al METAL CERAMICS PREPARED BY THE OXIDATION OF ALUMINUM POWDER UNDER HYDROTHERMAL CONDITIONS FOLLOWED BY THERMAL DEHYDRATION. II. COMPOSITION AND MICROTEXTURE OF THE COMPOSITES

S.F. Tikhov, V.I. Zaikovskii, V.B. Fenelonov, Yu.V. Potapova, V.N. Kolomiichuk, V.A. Sadykov

Kinetics & Catalysis, 41 (2000) pp. 835-843.

The microtexture of Al_2O_3/Al composites with different oxide contents formed in the hydrothermal treatment of aluminum followed by thermal decomposition of boehmite is examined by a set of adsorption and structural analysis techniques. Two main types of alumina microtexture are found: relatively loose agglomerates of amorphous particles and highly ordered aggregates of well-crystallized primary blocks of a larger size, the fraction of which increases with the oxide content of the composite leads to an increase in the fraction of micropores and a decrease in the fraction of mesopores. The mechanism of thermal decomposition of boehmite prepared by the hydrothermal oxidation of aluminum is refined.

REAL STRUCTURE OF METASTABLE FORMS OF ALUMINUM OXIDE

A.S. Ivanova, G.S. Litvak, G.N. Kryukova, S.V. Tsybulya, E.A. Paukshtis

Kinetics & Catalysis, 41 (2000) pp. 122-126.

Differences in the real structure of ν-Al_2O_3 samples obtained by the thermal decomposition of pseudoboehmite and boehmite prepared by the hydrothermal treatment of bayerite were found. The transformations of these structures during their conversion to δ-Al_2O_3 as the treatment temperature increased were studied. The rate of conversion of metastable alumina species into the stable α-Al_2O_3 phase significantly depends on the real structure of samples. The rate of this transformation is drastically retarded in the presence of extended defects in the oxides originated from boehmite, and the stability of metastable alumina species increased as the degree of surface dehydroxylation increased.

SUPPORT AND CATALYST FOR THE ALKYLATION OF BENZENE BY ETHYLENE PROCESS

R.A. Shkrabina, Z.R. Ismagilov, N.A. Koryabkina, Yu.K. Vorobiev

Euroasian J. Chem. Techn., 1 (2000) pp. 57-64.

A method for preparation of a spherical alumina support with preset porous structure for a catalyst of benzene alkylation with ethylene has been developed. The process of the support manufacture has been adjusted in a pilot installation, and an industrial installation for production of alumina support for the alkylation catalyst has been designed and built at the Shevchenko Plastics Plant (Aktau, Kazakhstan).

ROLE OF SILICA-ALUMINA CATALYST TEXTURE IN THE REACTION OF PROPANE OXIDATIVE DEHYDROGENATION IN THE PRESENCE OF SULFUR DIOXIDE

I.G. Danilova, A.S. Ivanova

Kinetics & Catalysis, 41 (2000) pp. 566-571.

The effects of preparation conditions, component ratio, and pretreatment temperature (1000–1550°C) of silica–alumina samples on their phase composition, texture characteristics, and catalytic properties are studied in the reaction of the oxidative dehydrogenation of propane by sulfur dioxide. It is shown that the samples contain individual silicon and aluminum oxides. The product of their interaction (mullite) is formed only at 1550°C. Mesoporous and macroporous catalysts with mono- and polydispersed pore distributions over sizes are obtained. It is found that the porous structure of the catalyst plays a key role in the process of the oxidative dehydrogenation of propane in the presence of sulfur dioxide at 600-700°C. The apparent rate of propylene formation increases with an increase in the pore volume with radii between 10 and 100 nm.

Propane is transformed into propylene more selectively on the catalyst where the pores with radii of 10–100 nm dominate; narrower pores (<10 nm) are favorable for the formation of coke and complete oxidation products.

HIGHLY-ORDERED ALUMINOSILICATE MESOPOROUS MESOPHASE MATERIALS: PHYSICO-CHEMICAL PROPERTIES AND CATALYTIC BEHAVIOUR

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J. Molec. Catal. A: Chemical, 158 (2000) pp. 349-354.

Structural and textural characteristics as well as coordination states of aluminium and some catalytic properties are studied for highly-ordered (with very narrow XRD reflections) aluminosilicate mesoporous mesophase materials (Si,Al)-MMM prepared with different aluminium concentrations by hydrothermal synthesis in the presence of $C_{16}H_{33}N(CH_3)_3Br$. As shown, all physico-chemical parameters measured for these systems including their structural hydrostability are strongly influenced by the aluminium content. Based on analysis of the results obtained, a description of probable transformations during formation of mesoporosity in the C_{16}-(Si,Al)-MMM is considered.

PHYSICOCHEMICAL AND CATALYTIC PROPERTIES OF $La_{1-x}Ca_x FeO_{3-0.5x}$ PEROVSKITES

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Kinetics & Catalysis, 41 (2000) pp. 287-292.

The phase analysis of $La_{1-x}Ca_xFeO_{3-0.5x}$ perovskites prepared by a ceramic process from oxides is studied by X-ray diffraction and differential dissolution methods. At x<0.5, the system does not form a continuous series of homogeneous solid solutions and does not consist of the members of a homological series. At x<0.5, the system contains two phases and calcium ferrite nanoparticles located on the surface of lanthanum ferrite. At x > 0.5, the formation of the structures of a brownmillerite-based homological series is found. The catalytic activity of perovskites depends nonmonotonically on the x value and reaches the maximum at x=0.6.

SYNTHESIS AND PHYSICOCHEMICAL AND CATALYTIC PROPERTIES OF PEROVSKITES $ABO_{3\pm y}$ (A=La, Sr, Ag; B= Mn, Co, Fe, Cu, Ti, Mo, V)

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Russ. J. Appl. Chem., 73 (2000) pp. 1383-1392.

The effect is considered exerted by synthesis conditions and composition of complex oxide materials $ABO_{3\pm y}$ based on *d* metals (Mn, Co, etc.) with perovskite structure on their catalytic activity in CO and *n*-heptane oxidation. The possibility of using such an empirical parameter as the content of active oxygen for prognosticating catalytic properties is evaluated. Neutron diffraction analysis was applied to determine the structure of the complex oxides and characteristics of particles of these materials.

MONOLITH HONEYCOMB MIXED OXIDE CATALYSTS FOR METHANE OXIDATION

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V.A. Sadykov, S.V. Tsybulya, V.A. Rogov,
A.N. Salanov

Stud. Surf. Sci. & Catal., Proceedings of the 12th International Congress on Catalysis, 130 (2000) pp. 3783-3788.

Low cost and active monolith catalysts for methane oxidation were developed. The preparation procedure includes the mechanochemical activation of mixed La-Ce rare-earth oxides and transition metal oxides, followed by their annealing, kneading with the binder, extrusion of plastic pastes, drying and calcination. In the temperature range of the methane + air mixture ignition (~ 500°C), the performance of optimized monolithic catalysts is mainly determined by their specific surface area controlled by the binder composition and preparation procedure.

OXIDATIVE DEHYDROGENATION OF PROPANE OVER MONOLITHS AT SHORT CONTACT TIMES

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I.A. Zolotarskii, N.A. Pakhomov, E.M. Moroz,
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Catal. Today, 61 (2000) pp. 93-99.

A specially designed tubular microreactor with independent control of feed preheat as well as catalyst temperature and allowing to rapidly quench reaction products was used to test performance of supported Pt-based monolithic catalysts in the reaction of propane oxidative dehydrogenation at short contact times. To minimize the impact of undesired homogeneous reactions capable to decrease propylene selectivity, proprietary straight-channel thin-wall high cell density corundum micromonoliths were chosen as supports. Catalytic properties of supported platinum were modified by using promoters known as dehydrogenation catalysts (tin, zinc aluminate spinel, transition metal pyrophosphates) as well as by tuning reaction mixture composition (propane/oxygen ratio, water and hydrogen content). In the operation temperature range up to 900^0C with contact times ~0.03-0.1 sec, ethylene/propylene selectivities were found to strongly depend upon the chemical composition of the active component and type of feed. The results thus obtained demonstrate that for Pt-based catalyts, propylene yield can be substantially improved by suppressing secondary reactions of deep oxidation and cracking.

DISTINCTIVE FEATURES OF SUPPORTED CATALYSTS PREPARED FROM PLATINUM CARBONYL CLUSTERS

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M.D. Smolikov

Kinetics & Catalysis, 41 (2000) pp. 720-728.

The formation of Pt/ν-Al_2O_3 and Pt/C catalysts from platinum carbonyl clusters $H_2[Pt_3(CO)_6]_n$ (n=2, 5) is studied. The strength of interaction between clusters (strong Lewis bases) and the support and the state of platinum in catalysts are governed by the acceptor strength of the support. The formation of a stable platinum compound with a surface of ν-Al_2O_3 (strong Lewis acid) is shown for a Pt/ν-Al_2O_3 catalyst by the method of radial distribution functions. In a Pt/C catalyst containing the same amount of Pt supported on a carbon material known to be a weaker acceptor, metallic platinum is formed along with surface-bonded platinum. Proceeding from the existence of the active phase of catalysts in the form of a surface platinum complex and platinum crystallites, the properties of catalysts are discussed in the complete oxidation of methane and the dehydrogenation of cyclohexane, as well as the high dispersity of platinum and its thermal stability.

PREPARATION OF THE Pd/C CATALYSTS: A MOLECULAR-LEVEL STUDY OF ACTIVE SITE FORMATION

P.A. Simonov, S.Yu. Troitskii, V.A. Likholobov

Kinetics & Catalysis, 41 (2000) pp. 255-269.

This review summarizes the results of molecular-level studies on the mechanism of Pd/C catalyst formation from the $PdCl_2$ precursor. Two processes occur in acidic media during the contact of H_2PdCl_4 with carbon: (a) adsorption of palladium chloride to form surface complexes and (b) redox interaction between $PdCl_2$ and carbon with the formation of palladium metal particles. The ratio between these adsorbed palladium species depends on the conditions of adsorption and especially on the size of carbon support grains and the oxidative atmosphere. The observations are explained by the fact that carbon support exhibits electrochemical and ligand properties. X-ray diffraction, X-ray scattering, XPS, and high-resolution electron microscopy revealed that the nanostructure of carbon materials, in particular the extent of their three-dimensional ordering, is crucial for the ligand properties. The presence of two forms, metallic and ionic, of sorbed palladium determines the bimodal size distribution of the metal. After the reduction of ionic species, metal particles are “blocked” with support. The nature of the ionic forms of palladium (mostly $(PdCl_2)_n$) clusters chemically and epitaxially bound to the carbon surface suggests the mechanisms of the bimodal distribution of the supported metal particles on the surface and the methods for the control of the ratio between “blocked,” low-dispersed, and highly-dispersed particles in the catalyst. One of these methods is the use of palladium polynuclear hydroxocomplexes (PHCs) with low oxidation potentials as starting compounds for catalysts preparation. The data on the PHC structure in a solution and its change upon the adsorption of PHC on the surface of the carbon material obtained by the ^{17}O, ^{23}Na, ^{133}Cs, and ^{35}Cl NMR techniques are discussed. PHCs are shown to be a clew of the $[Pd(OH)_2]_n$ polymeric filament, whose fractions are bound with alkali metal ions. When PHC is adsorbed on the surface of the carbon support and then dried, palladium oxide is formed from which highly dispersed metal particles are formed during reduction. The nature of alkali metal ions in PHC affects the activity of the Pd/C catalyst. An important role of the ligand, electrochemical, and lyophilic properties of carbon material during the formation of the species of the active catalyst component is discussed.

OXIDE CATALYSTS FOR AMMONIA OXIDATION IN NITRIC ACID PRODUCTION: PROPERTIES AND PERSPECTIVES

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Appl. Catal. A: General, 204 (2000) pp. 59-87.

This paper generalizes the results of long-term efforts aimed at research and development of industrial oxide catalysts for ammonia oxidation in the nitric acid production within two-bed (Pt gauzes + monolithic oxide layers) technology of the high pressure process.

Main factors determining performance of precious metals and oxides in the high-temperature ammonia oxidation are considered. The surface oxygen bonding strength determined by the surface atomic structure appears to be the most important. From this point of view, existing approaches to synthesis of mixed oxide systems including perovskites with controlled nitric oxide selectivity and good stability in the high-temperature process of ammonia oxidation are analyzed. Main features of the bulk oxide monolithic catalysts production technology and principles of a two-bed system design based upon the process mathematical modeling are briefly outlined. Proven economic benefits of this technology recently commercialized in Russia at nitric acid plants are debated.

FORMATION OF IMPERFECT MAGNESIUM OXIDE MODIFIED BY $Mg(NO_3)_2$ AND $LiNO_3$ AS PROBED BY IR SPECTRA

G.V. Odegova, N.A. Vasilieva

Russ. J. Inorg. Chem., 45 (2000) pp. 832-836.

The mechanism of formation of defect magnesium oxide during MgO hydration in solutions of $Mg(NO_3)_2$ and $LiNO_3$ is studied. An extraordinary compound whose bulk composition can be presented as $[Mg_{0.925}\square_{0.045}(N)_{0.03}]O_1$, is produced by solid-phase transformations in the products of MgO hydration in the $Mg(NO_3)_2$ solution. The defect magnesium oxide prepared in this manner is inhomogeneous both in structure and charge; it possesses high stability and is active in chain-radical reactions of hydrocarbon pyrolysis. In the $LiNO_3$ solution, the starting magnesium oxide hydrates only partly. The resulting defect $Mg(OH)_2$, which is modified by Li^+ and NO_3^- ions, also transforms to defect magnesium oxide upon calcining. The defect MgO prepared in this manner is less stable and transforms into ordinary magnesium oxide when exposed to the reaction medium.

FORMATION OF VANADIA-TITANIA OXIDE CATALYSTS

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Kinetics & Catalysis, 41 (2000) pp. 572-584.

The formation of vanadia–titania catalysts was studied with a complex of physicochemical methods. The use of highly dispersed anatase with a defect structure results in the formation of coherent boundaries of coalescence of the V_2O_5 and TiO_2 crystallites with the ratio V:Ti =1:1 in a wide range of vanadium and titanium concentrations. The catalysts containing coherent boundaries are active and selective in β-picoline oxidation to nicotinic acid.

SYNTHESIS AND STUDY OF ACID CATALYST 30%WO_3/SnO_2

G.M. Maksimov, M.A. Fedotov, S.V. Bogdanov, G.S. Litvak, A.V. Golovin, V.A. Likholobov

J. Molec. Catal. A: Chemical, 158 (2000) pp. 435-438.

Solid acid catalyst 30%WO_3/SnO_2 was synthesized and studied by IR, X-ray powder diffraction, solid state ^{117}Sn NMR and adsorbed pyridine thermodesorption. The catalyst consists of SnO_2 grains covered with W(VI) octahedra organized as in heteropolyacids. Its acidity is lower than the acidity of heteropolyacids but higher than that of the analogous catalyst WO_3/ZrO_2. The catalyst exhibits a high activity when used in the liquid phase acid-catalyzed reactions, but a part of it is washed out by polar solvents or substrates.

THE STRUCTURE OF THE VO_x OXO COMPLEXES ON THE SURFACE OF THE Al_2O_3 OF VARIOUS STRUCTURAL MODIFICATIONS

L.G. Simonova, O.B. Lapina, O.P. Krivoruchko, V.V. Terskikh

Kinetics & Catalysis, 41 (2000) pp. 270-275.

The structure of the surface VO_x oxo complexes prepared by deposition from aqueous solutions on alumina in various modifications (ν, η, χ, θ, and δ) is studied using ^{51}V and ^{1}H NMR. The crystal structure and acidic properties of the surface of the starting phases of Al_2O_3 do not substantially affect the structure of the surface VO_x compounds. This is explained by the reconstruction of the surface layer of the support and a change in its acidic properties caused by the action of impregnating aqueous solutions.

MECHANOCHEMICAL SYNTHESIS OF METASTABLE SOLID SOLUTIONS: PHASE COMPOSITION AND MICROSTRUCTURE EVOLUTION

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Inorg. Mater., 36 (2000) pp. 143-149.

The formation of Cu–Sn, Cu–In, Ni–Sn, and Ni-In supersaturated solid solutions during mechanochemical synthesis was studied. It was found that, in the process of synthesis, intermetallic compounds were formed first. Electron-microscopic examination revealed the presence of stacking faults and microstrains non-uniformly distributed in the initial stages of mechanochemical synthesis. Further mechanical activation makes the microstrain distribution more uniform. The microstructure of the metastable solid solutions is well described by models taking into account the major types of structural imperfections – second-order microstrains and deformation stacking faults.

THE SYNTHESIS OF COMPOSITES BY THE THERMOLYSIS OF THE SALTS OF CARBOXYLIC ACIDS

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Chem. for Sust. Development, 8 (2000) pp. 171-174.

The present paper deals with the thermal decomposition of the salts (both normal and acid) of transition metals with carboxylic acids: maleic, o-phthalic, and terephthalic. The residues after pyrolysis (up to 450°C) are composites including two structural components: an organic polymer matrix and spherical conglomerates from metal grains coated with polymer. Solid solutions of metal bimaleates have been synthesized, and their decomposition has been investigated. Some properties of resulting composites have been studied qualitatively.

SYNTHESIS AND STUDY OF PALLADIUM COLLOIDS AND RELATED CATALYSTS

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J. Molec. Catal. A: Chemical, 158 (2000) pp. 461-465.

Colloidal palladium particles were prepared by reduction with hydrogen of H_2PdCl_4 in a mixture of H_2O, trioctylamine (TOA), and cyclohexane. According to ^{14}N NMR, ^{35}Cl NMR and EXAFS data, the reduction of Pd was found to proceed under an auto-catalyzed regime via $(HTOA)_2[PdCl_4]$ complex formation. After complete reduction of Pd(II) (1 mol H_2 consumed per 1 Pd atom), H_2 consumption abruptly changed to 0.7 H_2 mol per 1 Pd atom. Unusually large amounts of H_2 absorbed per Pd-atom could be due to the formation of palladium hydride by highly dispersed and defected Pd particles. TEM shows that Pd particles in catalysts obtained by metal particle deposition on carbon material Sibunit look like “hedgehogs” with needles 100 Å long and 20-40 Å in diameter.

ANTISTATIC LATEX COATINGS BASED ON AMINE-CONTAINING COPOLYMERS

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Russ. J. Appl. Chem., 73 (2000) pp. 1798-1804.

Film-forming cationic amine-containing styrene-acrylate latexes with core-amine-containing shell particles were prepared. The influence of the latex composition and conditions of film formation on the antistatic properties of the resulting polymer coatings was examined. The surface resistivity ρ_s of the coatings is within 10^7-10^{11} Ω.

STUDIES OF X-RAY AMORPHOUS PHASE IN MECHANOCHEMICAL SYNTHESIS OF IRON SILICIDES FROM ELEMENTS

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J. Alloys & Compounds, 307 (2000) pp. 131-136.

Iron disilicide synthesis was developed by means of mechanochemical activation under intensive mechanical treatment. The X-ray amorphous phases formed during mechanical treatment of initial iron and silicon were investigated. The methods of the differential dissolution, differential thermal analysis and X-ray phase analysis were used. The formation of supersaturated amorphous solid solution of silicon in iron with limited concentration 17 at.% Si takes place during the initial period of activation. Primary phase obtained in this system is iron monosilicide formed in the decomposition of amorphous supersaturated solution.

REARRANGEMENTS OF SOME SESQUITERPENES OF THE AROMADENDRANE AND GUAIANE SERIES IN ACIDIC MEDIA

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Russ. J. Org. Chem., 36 (2000) pp. 40-54.

(+)-Ledene and (+)-aromadendrene undergo rearrangements in various acidic media (HSO_3F-SO_2FCl, HCOOC, and over TiO_2/SO_4^{2-}) to give new tricyclic and spirocyclic compounds. Under the same conditions structurally related (-)-isoledene and (+)-γ-gurjunene give rise to mixtures of bicyclic dienes having a guaiane skeleton. The experimental data are discussed with regard to the results of computer simulation of the most favorable transformation pathways by molecular-mechanics and quantum-chemical methods.

FORMATION OF BIMETALLIC Pt-Rh SURFACE WITH NANOSIZE METAL DOMAINS

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React. Kinet. & Catal. Lett., 72 (2000) pp. 163-168.

An approach to produce a bimetallic Pt-Rh model catalyst has been developed. It includes vacuum deposition of platinum on a Rh_2O_3 film, followed by the oxide reduction with hydrogen. The thermal stability range of the resulting bimetallic structure has been determined.

GROWTH AND CHARACTERIZATION OF $LiInS_2$ SINGLE CRYSTALS

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J. Cryst. Growth, 218 (2000) pp. 313-321.

Bulk $LiInS_2$ single crystals were grown using the Bridgman-Stockbarger technique. The crystals were characterized in composition, structure and defects. The composition was determined both in average and local versions, the latter was carried out using the unique differential dissolution technique. For all crystals a departure from ideal $LiInS_2$ stoichiometry, especially for cations, was detected. In the optical absorption spectra a strong band at 360 nm which disappears after annealing in S_2 vapor was, with a high probability, related to sulfur vacancies *V*s: their oscillator strength is f ≥ $1.3 \cdot 10^{-4}$. The blue photoluminescence in all crystals is likely to be due to In_{Li} antisite defect with an energy level 0.62 eV below the condition band. The universal values of forbidden band gap, E_g are 3.72 and 3.57 eV at 80 and 300 K, respectively, for all crystals studied indicating the similar character of dominant bonds.

CONSOLIDATION OF METAL OXIDE NANOCRYSTALS. REACTIVE PELLETS WITH CONTROLLABLE PORE STRUCTURE THAT REPRESENT A NEW FAMILY OF POROUS, INORGANIC MATERIALS

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J. Amer. Chem. Soc., 122 (2000) pp. 4921-4925.

Nanocrystals of MgO (4 nm) exist as polyhedral structures with high surface concentration of edge/corner sites. In powder form the crystallites weakly agglomerate into porous weblike structures of ~1400 nm according to small-angle X-ray scattering. Upon consolidation of these fine powders under pressure, pellets can be readily prepared that maintain their high surface areas, and small crystallite sizes. Large pore volumes and pore size openings can be controllably decreased with pelletization pressure increase. The pellets retain their voracious adsorbent affinities and capacities for a wide variety of organic molecules and acid gases. Quantum measurements on the adsorption of alcohols **vs**. pelletization pressure reveal a pattern of molecule size selectivity.

EFFECTIVE CATALYSTS FOR DIRECT CRACKING OF METHANE TO PRODUCE HYDROGEN AND FILAMENTOUS CARBON: PART I. NICKEL CATALYSTS

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Appl. Catal. A: General. 201 (2000) pp. 61-70.

Data obtained by studying model catalytic systems were used to develop high-loaded nickel catalysts for direct cracking of methane into hydrogen and catalytic filamentous carbon (CFC). The approach to the synthesis of these catalysts can be the basis for development of catalytic nickel systems for commercial processing of natural gas. The catalysts were synthesized by fusing nickel nitrate with zirconium nitrate, or nickel nitrate with copper-doped aluminium nitrate followed by decomposition of the mixture at 300–450°C and its additional stabilization by silica. The silica textural promoter was formed by thermal decomposition of polyethoxysilane introduced into pores of the oxide matrix. The catalysts reduced by hydrogen comprised nickel in the amount of 85–90%. Unlike preparation of co-precipitated systems, synthesis of the catalysts mentioned does not include stages of filtration and wastewater treatment. Principal characteristic of the catalysts' effectiveness for the reaction of decomposition of methane, i.e. carbon yield per gram of nickel, of the suggested systems was close or superior to that achieved before using the best nickel or nickel–copper catalysts prepared by co-precipitation.

PLASMOCHEMICAL SYNTHESIS OF THIN FILMS OF SILICON CARBONITRIDE FROM DIMETHYL(2,2-DIMETHYLHYDRAZINO)SILANE

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Chemistry for Sustainable Devel., 8 (2000) 731-738.

Ecologically friendly process for plasmochemical deposition of thin films of silicon carbonitride from new compound – dimethyl(2,2-dimethylhydrazino)silane (DMDMHS) – is discussed. DMDMHS is a product of processing of rocket propellant, asymmetric dimethylhydrazine (heptyl). Dependencies of the film chemical composition on the synthetic conditions were studied. Possibility to control characteristics of the synthesized layers through variation of the process parameters was demonstrated. Mechanisms of plasmochemical and heterophase transformations of DMDMHS to form silicon carbonitride films were suggested. The films were shown to be substoichiometric SiN_x consisting of incomplete SiN tetrahedron with a part of nitrogen sites occupied by carbon. The ratio of Si–N/Si–C bonds in the material was determined by the temperature of synthesis at other stable parameters.

Catalysis on Zeolites and Zirconia-Based Materials

MECHANISM OF COKE INFLUENCE ON THE CATALYTIC ACTIVITY OF FEZSM-5 IN THE REACTION OF BENZENE OXIDATION INTO PHENOL

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Kinetics & Catalysis, 41 (2000) pp. 771-775.

The influence of coke formation in the reaction of benzene oxidation by nitrous oxide into phenol on the catalytic activity and concentration of iron-containing active sites (α-sites), which are stabilized in the microporous structure of FeZSM-5 zeolite, is studied. The deactivation by coke is explained by the poisoning of α-sites, whose concentration decreases linearly with an increase in the coke content, rather than by the blocking of zeolite pores. The activity per one α-site remains unchanged. This fact indicates the absence of diffusion limitations associated with coke formation. The toxicity of coke for the α-sites is determined. The coke amount equivalent to 100–120 benzene molecules is shown to result in the deactivation of one active site.

ROOM-TEMPERATURE OXIDATION OF HYDROCARBONS OVER FeZSM-5 ZEOLITE

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Stud. Surf. Sci. & Catal.,
Proceedings of the 12th International
Congress on Catalysis,
130 (2000) pp. 875-880.

Interaction of a variety of organic molecules with α-oxygen formed by N_2O decomposition over FeZSM-5 zeolites leads to products of selective hydroxylation. O-insertion occurs rapidly at room temperatures and affects both aromatic and aliphatic C-H bonds.

MOLECULAR DYNAMICS OF ISO-BUTYL ALCOHOL INSIDE ZEOLITE H-ZSM-5 AS STUDIED BY DEUTERIUM SOLID STATE NMR

A.G. Stepanov, M.M. Al'kaev, A.A. Shubin

J. Phys. Chem. B., 104 (2000) pp. 7677-7685.

The molecular mobility of *iso*-butyl alcohol, selectively deuterated in the methylene group (iBA[1-d_2]) or in the methyl groups (iBA[3-d_6]), adsorbed on zeolite H-ZSM-5 was studied with ^{2}H NMR. At 115-293 K ^{2}H NMR line shape for the adsorbed iBA[3-d_6] represents a superposition of one solid-like and two liquid-like signals, while for iBA[1-d_2] it is a superposition of the solid-like and the liquid-like lines. Two liquid-like signals are assigned to the alcohol molecules isotropically reorienting with the correlation time $\tau_R \sim 1 \times 10^{-6}$s by jumping among Al-OH-Si groups, located inside the channels and at channel intersections of the zeolite channel system. Being adsorbed on Al-OH-Si groups these two types of the alcohol molecules differ by the effective amplitude of libration γ_0 (γ_0 is a libration cone semiangle) of the methyl groups, which is large for both adsorption sites ($\gamma_0 \sim 52°$ for one of the types and $\gamma_0 \sim 72°$ for the other one). The solid-like signal with the observed quadrupole splitting of 38 kHz is assigned to the alcohol molecules located inside the zeolite channels. These alcohol molecules reorient with $\tau_R > 4.2 \times 10^{-6}$s and their methyl groups experience small librations with amplitude $\gamma_0 \sim 19°$. Methyl groups of the alcohol molecules located at channel intersections rotate about CH_3-CH axis with correlation time $\tau_P = (1.4 - 2.6) \times 10^{-11}$s at 293 K and activation energy $E_P = 11 - 12$ kJ/mol, while those located inside the channel rotate with the correlation time $\tau_j \sim 2 \times 10^{-10}$s at 293 K and activation energy $E_j = 10.5$ kJ/mol. The difference in the rotation rates is attributed to the influence of the walls of the zeolite channel on dynamics of one axis methyl group rotation, which is expected to be more profound in the confined area of a narrow channel than at channel intersection.

ALKANE CARBONYLATION WITH CARBON MONOXIDE ON SULFATED ZIRCONIA. NMR OBSERVATION OF KETONE AND CARBOXYLIC ACID FORMATION FROM ISO-BUTANE AND CO

A.G. Stepanov, M.V. Luzgin, A.V. Krasnoslobodtsev,
V.P. Shmachkova, N.S. Kotsarenko

Angew. Chem., Int. Ed., 39 (2000) pp. 3658-3660.

Iso-butane undergoes carbonylation by CO on sulfated zirconia catalyst at 70°C as has been shown by *in situ* solid state ^{13}C NMR, *ex situ* ^{13}C high resolution NMR and GC-MS analyses. Methyl *iso*-propyl ketone selectively forms in the absence of water, while pivalic acid represents the primary reaction product in the presence of coadsorbed water.

FORMATION OF CARBOXYLIC ACIDS FROM SMALL ALKANES IN ZEOLITE H-ZSM-5

M.V. Luzgin, A.G. Stepanov, A. Sassi*, J. Sommer*
(*Universite Louis Pasteur, Strasbourg, France)

Chem. Eur. J., 6 (2000) pp. 2368.

The activation of propane and *iso*-butane in acidic zeolite H-ZSM-5 in the presence of both CO and H_2O has been studied by *in situ* solid state NMR and GC analysis. Evidence was provided that at 373-473 K propane converts via C-C bond cleavage to produce *iso*-butyric acid with evolution of both methane and ethane. *Iso*-butane was transformed into pivalic acid with simultaneous production of hydrogen. The low conversion (1-2%) at this temperature was rationalized by the existence of a small number of sites capable of generating carbenium ions which are trapped by CO at this temperature. A formate species was observed when CO and H_2O were present on H-ZSM-5, which disappeared in the presence of the alkane. At 573 K the generation of large amounts of CO_2 indicates a much higher conversion of the alkanes in carboxylic acids which decompose, however, under the reaction conditions.

FORMATION OF CARBOXYLIC ACIDS FROM SMALL ALKANES IN ZEOLITE H-ZSM-5

A.G. Stepanov, M.V. Luzgin, A. Sassi*, J. Sommer* (*Universite Louis Pasteur, Strasbourg, France)

Proceedings of the 12th International
Congress on Catalysis,
CD ROM, RR099

The activation of propane and *iso*-butane in acidic zeolite H-ZSM-5 in the presence of both CO and H_2O has been studied by *in situ* solid state NMR and GC analysis. Evidence was provided that at 373-473 K propane converts via C-C bond cleavage to produce *iso*-butyric acid with evolution of both methane and ethane. *Iso*-butane was transformed into pivalic acid with simultaneous production of hydrogen. The low conversion (1-2%) at this temperature was rationalized by the existence of a small number of sites capable of generating carbenium ions which are trapped by CO at this temperature.

ADVANCES IN OXIDATION CATALYSIS: BENZENE OXIDATION TO PHENOL WITH NITROGEN MONOXIDE

G.I. Panov, A.S. Kharitonov

Russ. Chemical J., XLIV (2000) pp. 7-18.

The paper presents a review of the field of oxidative catalysis related to the reactions of oxidative hydroxylation of paraffines and aromatics for production of different alcohols and phenols. At present they are produced by complex multistage reactions. The different ways for this problem solving are analyzed based on the reaction of benzene oxidation to phenol. Main attention is paid to a new concept of benzene to phenol oxidation, which became possible due to the discovery of novel catalytic system FeZSM-5 - N_2O. The properties of this system are similar to those of natural enzymes monooxygenases.

THE Fe ACTIVE SITES IN FeZSM-5 CATALYST FOR SELECTIVE OXIDATION OF CH_4 TO CH_3OH AT ROOM TEMPERATURE

N.S. Ovanesyan*, K.A. Dubkov, A.A. Pyalling*, A.A. Steinman* (*Institute of Chemical Physics, Chernogolovka, Russia)

J. Radioanal. & Nuclear Chemistry, 246 (2000) pp. 149-152.

Change of valent state of Fe ions of α-centers at α-oxygen generation from N_2O and subsequent its interaction with methane and hydrogen are studied with Mössbauer spectroscopy. α-Centers represent out-of-lattice iron complexes in oxidation state 2+. The localization of α-oxygen is accompanied by oxidizing transition Fe^{2+} to Fe^{3+} in active center. After the reaction of α-oxygen with methane or hydrogen the reverse reduction Fe^{3+} to Fe^{2+} is observed, but this process is not completely reversible.

SOME PROCEDURES OF OLIGOMERIZATION OF α-METHYLSTYRENE

V.P. Talzi, V.P. Doronin, T.P. Sorokina, S.V. Ignashin

Russ. J. Appl. Chem., 73 (2000) pp. 835-838.

The use of zeolites Y with various Brönsted acidity and also methylene chloride as a solvent for production of α-methylstyrene dimer, used as a chain-terminating agent in polystyrene production, was studied.

THE MICROSTRUCTURE AND PROPERTIES OF FRAMEWORK ZIRCONIUM PHOSPHATES BASED NANOCOMPOSITES - CATALYSTS OF ALKANE ISOMERIZATION

V.A. Sadykov, S.N. Pavlova, G.V. Zabolotnaya, R.I. Maksimovskaya, D.I. Kochubey, V.V. Kriventsov, G.V. Odegova, N.M. Ostrovskii, S.V. Tsybulya, E.B. Burgina, V.I. Zaikovskii, M.V. Chaikina*, V.V. Lunin, R. Roy***, D. Agrawal***** (*Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia; **Moscow Lomonosov State University, Moscow, Russia; ***Materials Research Lab., Penn State University, USA)

Mat. Res. Innov., 3 (2000) pp. 276-285.

Nanocomposites based upon framework zirconium phosphates with supported WO_3, MoO_3 and Pt nanoparticles were synthesized via the incipient wetness impregnation of high-surface-area mesoporous phosphate samples with water solutions of corresponding salts followed by drying and calcination. The structure and surface properties of nanocomposites were studied by using combination of structural and spectral methods. Due to a strong interaction between supports and supported species, the structure of the latter differs considerably from that of the bulk phases. Surface acid centers typical for zirconium phosphates disappear suggesting their participation in bonding nanoparticles of promoters. Instead, new types of strong acid sites associated with tungsten oxide clusters emerge. The effect of these promoters on performance of zirconium phosphates in the reaction of pentane and hexane isomerization is considered.

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Mat. Res. Soc. Symp. 581 (2000) pp. 315-320.

The structure and surface properties of composites based upon high-surface-area framework zirconium phosphates with supported WO_3, MoO_3 and Pt nanoparticles were studied by using combination of structural and spectral methods. The effect of these promoters on performance of zirconium phosphates in the reaction of pentane and hexane isomerization is considered.

THE NOVEL ACID CATALYSTS - FRAMEWORK ZIRCONIUM PHOSPHATES: THE BULK AND SURFACE STRUCTURE

S.N. Pavlova, V.A. Sadykov, G.V. Zabolotnaya, D.I. Kochubey, R.I. Maksimovskaya, V.I. Zaikovskii, V.V. Kriventsov, S.V. Tsybulya, E.B. Burgina, A.M. Volodin, E.A. Paukshtis, M.V. Chaikina*, N.N. Kuznetsova, V.V. Lunin**, D. Agrawal***, R. Roy*****
(*Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia; **Moscow Lomonosov State University, Moscow, Russia; ***Penn State University, USA)

J. Molec. Catal. A: Chemical, 158 (2000) pp. 319-323.

Framework zirconium phosphates structural features and surface properties were studied and compared with catalytic performance in the reactions of hexane isomerization. Isomerization activity of cubic or rhombohedral zirconium phosphates samples correlates with the density of the strongest Lewis centers probed by TEMPON test molecule.

HIGHLY DISPERSED FRAMEWORK ZIRCONIUM PHOSPHATES - ACID CATALYSTS FOR PENTANE AND HEXANE ISOMERIZATION

S.N. Pavlova, V.A. Sadykov, G.V. Zabolotnaya, R.I. Maksimovskaya, D.I. Kochubey, V.V. Kriventsov, N.M. Ostrovskii, S.V. Tsybulya, E.B. Burgina, V.I. Zaikovskii, M.V. Chaikina*, V.V. Lunin, R. Roy***, D. Agrawal*****
(*Institute of Solid State Chemistry, Novosibirsk, Russia; **Moscow Lomonosov State University, Moscow, Russia; ***Penn State University, USA)

Stud. Surf. Sci. & Catal.,
Proceedings of the 12th International Congress on Catalysis, 130 (2000) pp. 2399-2404.

The structural features, texture and surface properties of highly dispersed partially substituted framework zirconium phosphates synthesized via sol-gel or mechanochemical activation route followed by the hydrothermal treatment in the presence of polyethylene oxide were studied and compared with catalytic properties in the pentane and hexane isomerization. The most efficient promoter was found to be Si which increases the surface density of the Brönsted Zr-OH centers. Pt-supported Si-modified systems demonstrate promising activity and selectivity in propane and hexane hydroisomerization at 300-400°C.

PREPARATION OF FINE-PARTICLE ZIRCONIA-BASED MATERIALS

A.S. Ivanova, M.A. Fedotov, G.S. Litvak, E.M. Moroz

Inorg. Mater., 36 (2000) pp. 352-358.

The influence of the synthesis conditions, the nature of the added component, and its concentration on the formation of fine-particle M–Zr–O (M=Fe, Y, La) materials was studied in the temperature range 383–973 K. The materials prepared at a variable pH of precipitation and containing 2–33 mol % M_2O_3 were X-ray amorphous in the range 383–673 K, except for the Fe–Zr–O samples with 33 mol % Fe_2O_3, which contained α-Fe_2O_3 . Heat treatment at 973 K resulted in the formation of a *c*-ZrO_2-based solid solution, whose lattice parameter depended on the nature and concentration of the second component. The minimum particle size of the materials studied was 2.5–12 nm in the range 383–673 K and 3–47 nm at 973 K.

ZIRCONIUM-CONTAINING COMPOSITIONS WITH A COMPONENT RATIO CHARACTERISTIC OF THE GARNET STRUCTURE: PHYSICOCHEMICAL AND CATALYTIC PROPERTIES

A.S. Ivanova, M.V. Mikhan', G.M. Alikina, G.S. Litvak, E.M. Moroz, E.B. Burgina

Kinetics & Catalysis, 41 (2000) pp. 816-825.

The possibility for the formation of garnet structures in the Mn–Fe–Zr–O and Ca–Sm–Zr–O systems obtained by the precipitation of the corresponding salts is studied. It is shown that, in the Mn–Fe–Zr–O system, garnet is crystallized at 860-920°C, for which probable cation distribution is estimated to be $\{Zr_{2.5}^{4+}Mn_{0.5}^{2+}\}[Mn_2^{2+}](Fe_{2.5}^{3+}Mn_{0.5}^{3+})O_{12}$. In the Ca–Sm–Zr–O system, the perovskite $CaZrO_3$, pyrochlore $Sm_2Zr_2O_7$, and CaO are formed at 900–1200°C, but compounds with garnet structures are not found. The reported systems are characterized by surface areas of 300–450 m^2/g at 450°C, and they have the polydisperse distribution of pores over sizes. The introduction of surfactants at the stage of component mixing enables an increase in the overall pore volume and mechanical strength of these systems. The Mn–Fe–Zr and Ca–Sm–Zr compositions are active catalysts for the complete oxidation of hydrocarbons.

FORMATION OF THE PORE STRUCTURE OF ZIRCONIUM DIOXIDE AT THE STAGE OF GEL AGING

V.Yu. Gavrilov, G.A. Zenkovets

Kinetics & Catalysis, 41 (2000) pp. 561-565.

The formation of the pore structure of zirconium dioxide at the gel aging stage in an intermicellar medium is studied. The processes, which occur in the course of aging, and the features of the structure formed depend on the pH of gel precipitation. The calcination of ZrO_2 at 500°C is accompanied by the diffusion process of bulk sintering, which results in a substantial reconstruction of the pore space of the xerogel.

STUDY OF ZIRCONIA MICROPOROUS STRUCTURE

V.Yu. Gavrilov

Kinetics & Catalysis, 41 (2000) pp. 715-719.

The microporous structure of zirconium dioxide obtained by precipitation at different pH and different times of gel aging is studied by the physical adsorption of nitrogen, oxygen, and molecular hydrogen. It is shown that the ratio between the supermicropore surface areas measured by the adsorption of O_2 and N_2 as a function of the supermicropore volume previously revealed for SnO_2 is also retained for zirconia (the surface area of supermicropores measured by O_2 adsorption is larger than that measured by N_2 adsorption). Possible reasons for this phenomenon are discussed. The conclusions on the factors responsible for the formation of the zirconia microporous structure are drawn.

ACIDIC PROPERTIES OF SULFATED ZIRCONIA

E.A. Paukshtis, V.P. Shmachkova, N.S. Kotsarenko

React. Kinet. & Catal. Lett., 71 (2000) pp. 385-392.

IR spectroscopy of adsorbed probe molecules (CO, pyridine) is used to characterize the acidic properties of sulfated zirconia derived from zirconium oxide and hydroxide. Their acidic properties are found to be similar. The strength of the Lewis and Brönsted sites measured by the frequency shift of adsorbed CO is lower than that in zeolites. It is concluded that sulfated zirconia have no superacid Brönsted and Lewis sites. Brönsted sites capable of protonating pyridine vanish when calcining the catalysts at temperature above 773 K, but the strength and concentration of the Lewis acid sites do not change.

UNUSUAL MANIFESTATION OF BENZENE RADICAL CATIONS IN ESR SPECTRA ON SULFATED ZIRCONIA

A.F. Bedilo, A.M. Volodin

J. Molec. Catal. A: Chemical, 158 (2000) pp. 405-408.

A narrow singlet has been observed in the ESR spectra after benzene adsorption on sulfated zirconia, with its evacuation and freezing leading to the reversible formation of benzene dimer radical cations. The singlet has been proposed to result from the delocalization of the electron density throughout several benzene rings due to fast electron exchange. This distinguishes sulfated zirconia catalysts from zeolites where this effect is not observed because of the small size of channels.

DEVELOPMENT OF AN ESR TECHNIQUE FOR TESTING SULFATED ZIRCONIA CATALYSTS

A.F. Bedilo, A.S. Ivanova, N.A. Pakhomov,
A.M. Volodin

J. Molec. Catal. A: Chemical, 158 (2000) pp. 409-412.

Sulfated zirconia catalysts active in the isomerization of n-butane have been synthesized by sulfating crystalline monoclinic and cubic zirconia supports precalcined at 700°C. Strong acceptor sites capable of ionizing chlorobenzene have been observed on all active catalysts irrespective of the crystalline structure. A simple instrumental technique based on the chlorobenzene adsorption has been suggested for probing sulfated zirconia catalysts.

FORMATION OF TETRAMETHYLETHYLENE RADICAL CATIONS AFTER PENTANE ADSORPTION ON SULFATED ZIRCONIA

A.F. Bedilo, A.V. Timoshok, A.M. Volodin

Catal. Lett., 68 (2000) pp. 209-214.

Tetramethylethylene radical cations have been registered by ESR after pentane adsorption on sulfated zirconia. The radical cations proved to be not stable in the presence of oxygen, only molecular oxygen radical anions being registered. Tetramethylethylene formation and pentane disproportionation are shown to occur under illumination within the same spectral region proving that the former is formed as a side product of pentane transformations.

ESR STUDY OF MONOMER ND TRIPLET DIMER NO ADSORBED ON SULFATED ZIRCONIA

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M. Shiotani[b], **A. Lund**[a] ([a]Linkoping University, Linkoping , Sweden; [b]Hiroshima University, Higashi-Hiroshima, Japan)

Chem. Phys. Lett, 327 (2000) pp. 165-170.

Triplet state NO dimers stabilized on the surface of sulfated zirconia ($g_\perp$ = 1.993, $g_{||}$ = 1.942, $D_\perp$ = 195 G, E ≈ 0) have been observed by ESR. They are formed by the adsorption of NO molecules on pair (acceptor) surface sites represented, most likely, by two adjacent (d = 5.2 Å) low-coordinated Zr^{4+} ions. A new single line (Lorentz line with g = 1.993 and line width 18 G) of NO monomers adsorbed on active sites of sulfated zirconia has been observed. The sites where this form is stabilized seem to be very strong acceptors responsible for the formation of radical cations after adsorption of aromatic molecules.

INFLUENCE OF THE NATURE OF COMPONENTS IN MECHANICALLY ACTIVATED MIXTURE OF ZIRCONIUM ON SILICON OXIDES ON SOLID-PHASE SYNTHESIS OF ZIRCON

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E.S. Stoyanov, M.V. Povetkina,**
A.M. Chekmarev, V.L. Shafirov**,**
O.B. Vinokurova** (*Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia; **Mendeleev Russian University of Chemical Engineering, Moscow, Russia)

Russ. J. Appl. Chem., 72 (1999) pp. 1498-1502.

The effect of hydration of zirconium and silicon oxides on solid-phase synthesis of zircon $ZrSiO_4$ with mechanical activation of their equimolar mixture and subsequent calcination at 1200°C was studied. The optimal composition of the oxides, ensuring the maximum yield of zircon, was determined.

Studies on Silver Catalysts

ASSOCIATIVE OXYGEN SPECIES ON THE OXIDIZED SILVER SURFACE FORMED UNDER O_2 MICROWAVE EXCITATION

A.I. Boronin, S.V. Koshcheev, K.T. Murzakhmetov, V.I. Avdeev, G.M. Zhidomirov

Appl. Surf. Sci., 165 (2000) pp. 9-14.

The experimental methods of photoelectron spectroscopy (XPS, UPS) and the quantum mechanical calculations are applied for analysis of oxygen states on the silver oxide surface. At low temperatures ($T < 470$ K) the silver surface is intensively oxidized by a microwave oxygen discharge to form cuprite Ag_2O. Two adsorbed oxygen species of the atomic (dissociative) and molecular (associative) nature can be adsorbed on the cuprite Ag_2O surface. A comparison of the UPS data and the DFT calculations of molecular models Ag2-O_2 and Ag2-O_3 shows that the formation of ozonide-like structures is preferable to that of peroxide species. Thermal stability and the reaction probability of the adsorbed states are investigated.

QUASIMOLECULAR STABLE FORMS OF OXYGEN ON SILVER SURFACE. THEORETICAL ANALYSIS BY THE DENSITY FUNCTIONAL THEORY METHOD

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

J. Molec. Catal. A: Chemical, 154 (2000) pp. 257-270.

A quantum chemical investigation of possible associative oxygen forms of oxygen on defective silver surface has been performed with the use of gradient corrected density functional theory (DFT) in the cluster approximation. A surface defect was simulated by a cation vacancy (V). Cluster models (M1: Ag12 and M2: O3Ag12) of an active adsorption site (AS) with a vacancy were chosen on the basis of the structure of high-temperature layered silver oxide. The adsorbed layer on the defective surface was simulated by three oxygen atoms. For the atomic and associative (molecular) forms, the computations gave two stable structures of the adsorbed layer with C_{3V} and C_{2V} symmetry. The quasimolecular C_{2V} structure -Ag-O-O_{ep}-O-Ag- resembling metal ozonides is by 44 kcal/mol more stable than the atomic C_{3V} structure. The C_{2V} structure is singlet and has an electrophilic epoxidizing oxygen atom O_{ep}. A theoretical estimation of the density of states (DOS) in the quasimolecular oxygen form revealed a complex structure below the 4d band. Additional DOS peaks in this region are due to associative O-O bonds.

PHYSICOCHEMICAL INVESTIGATION OF THE COPPER AND SILVER CATALYSTS OF THE ETHYLENE GLYCOL OXIDATION

O.V. Vodyankina*, S.V. Koshcheev, V.T. Yakushko, A.N. Salanov, A.I. Boronin, L.N. Kurina* (*Tomsk State University, Tomsk, Russia)

J. Molec. Catal. A: Chemical, 158 (2000) pp. 381-387.

The copper and silver catalysts of ethylene glycol oxidation into glyoxal have been investigated by means of XPS, SEM and TGA methods. The data presented in this work show that two types of the carbon deposits, which accompany glyoxal synthesis, are formed. First type of deposits are the graphite-like structures which can be formed on Cu surface at lean content of oxygen in the reaction mixture. Second type of deposits is the oxycarbon structure which grows as filaments. Both morphology and the chemical composition of oxycarbon deposits depend strongly on the reaction mixture. Oxygen in the reaction mixture leads to the predominant formation of the oxycarbon filaments on the oxidized metal surface.

GLYOXAL SYNTHESIS BY VAPOUR–PHASE ETHYLENE GLYCOL OXIDATION ON A SILVER AND COPPER CATALYSTS

O.V. Vodyankina*, L.N. Kurina,* A.I. Boronin, A.N. Salanov (*Tomsk State University, Tomsk, Russia)

Stud. Surf. Sci. & Catal.,
Proceedings of the 12th International Congress on Catalysis, 130 (2000) pp. 1775-1680.

The data presented in this work show that efficiency of supported Ag catalysts is associated with the stabilization of active component in the high – dispersity $Ag^{+\delta}$ state under the influence of oxygen of the support lattice. However, uncovered by Ag lots of catalyst surface is answerable for unselective ethylene glycol oxidation. The application of the double-layer Cu-Ag catalytic system increases the selectivity of the ethylene glycol oxidation into glyoxal. One of the main reasons is the growth of efficiency of Cu layer located in the field of reactor where more low oxygen concentration and temperature in comparison with Ag layer take place. One can assume that the coke deposition on the oxidized metal catalyst surface exert favorable influence on selectivity of the major process. The coke deposits are the oxycarbon structures which grow as filaments. It is proposed the destruction of oxycarbon layer under the oxygen action leads to the glyoxal appearance in the reaction products.

Studies on Silica Materials

THE KINETIC MODEL OF DISSOLUTION OF SILICON DIOXIDE AEROGELS IN AN AQUEOUS NaOH SOLUTION

S.A. Shaurman*, A.G. Okunev*, A.F. Danilyuk, Yu.I. Aristov (* Novosibirsk State University, Novosibirsk, Russia)

Colloid J., 62 (2000) pp. 502-508.

Plausible explanations for previously obtained kinetic data on the dissolution of silicon dioxide aerogels in an aqueous 0.05 M NaOH solution in the temperature range 15–37°C were considered. Because the coincidence of specific surface areas measured by the BET and small-angle X-ray scattering techniques suggests an absence of closed pores in the structure of investigated aerogels, the heterogeneity of their surfaces was considered to be the most probable reason for the variations in the shape of kinetic curves. A model of dissolution was proposed. The model is based on the assumption of two kinetically nonequivalent types of surface atoms (inactive and active) and takes into account finite sizes of these atoms. The model is a modification of the known Delmon model and uses a parameter E_s having a simple physical meaning of the initial number of active sites of dissolution on a primary aerogel particle. The activation energy of dissolution (80±6 kJ/mol) and the interfacial energy (0.09 and 0.24 J/m^2 for coarsely and finely dispersed samples, respectively) were obtained by approximating experimental data by calculated dissolution curves. It was shown that the number of active sites, E_s, increases linearly with the radius of primary particles.

KINETICS OF THE GROWTH OF SUPRAMOLECULAR CRYSTALS IN A SUSPENSION OF MONODISPERSED SPHERICAL SILICA PARTICLES

V.V. Serdobintseva*, A.F. Danilyuk, D.V. Kalinin (*Institute of Mineralogy and Petrography, Novosibirsk, Russia)

React. Kinet. & Catal. Lett., 71 (2000) pp. 93-98.

Kinetics of the supramolecular crystallization of monodispersed spherical silica particles (MSSP) suspension in diethyl ether with close to the phase transition point concentration of structural units has been studied for the first time. It was found that the linear crystal growth rate depends on temperature and the process activation energy is 25 kcal/mol. The linear law of the crystal growth is associated with diffusion of the structural units on the interface.

MECHANISM OF THE FORMATION OF POROUS SILICATE MESOPHASES

V.N. Romannikov, V.B. Fenelonov, A.V. Nosov, A.Yu. Derevyankin, S.V. Tsybulya, V.N. Kolomiichuk

Kinetics & Catalysis, 41 (2000) pp. 108-115.

The formation of mesoporous mesophase systems prepared by precipitation of soluble forms of SiO_2 at the surface of micelles of cetyltrimethylammonium cations was examined. A molecular mechanism of the formation of a silicate coating and a macroscopic mechanism of the formation of a mesophase were found and discussed. A combination of these mechanisms describes the processes proceeding during the synthesis. It can also explain the observed changes in the structure and texture characteristics of the mesophase.

SYNTHESIS OF HIGH SURFACE AREA SILICA GELS USING POROUS CARBON MATRICES

M.A. Ermakova, D.Yu. Ermakov, G.G. Kuvshinov, V.B. Fenelonov, A.N. Salanov

J. Porous Mater., 7 (2000) pp. 435-441.

Porous silica was prepared using the sol-gel synthesis with porous carbon matrices as a pore-forming support. Tetraethoxysilane (TEOS) was hydrolyzed in an acid medium in the presence of a substoichiometric amount of water. Various carbon materials were used, among them Sibunit and catalytic filamentous carbon. Carbon matrices were impregnated with hydrolyzed TEOS and dried, then carbon was removed by burning out in air at 873 K. The obtained porous silica samples were studied by adsorption and electron microscopic methods. The specific surface area as high as 1267 m^2/g and pore volume as high as 5.7 cm^3/g were determined for some silica samples. Thus deposited SiO_2 was found to cover the carbon surface copying its surface. With

CFC used as carbon matrix, silica nanotubes were obtained. Thermostability of such silica is significantly greater as compared to silica gels reported earlier.

FILAMENTOUS CARBON TEMPLATED SiO_2-NiO AEROGEL: STRUCTURE AND CATALYTIC PROPERTIES FOR DIRECT OXIDATION OF HYDROGEN SULFIDE INTO SULFUR

M.A. Ermakova, D.Yu. Ermakov, M.Yu. Lebedev, N.A. Rudina, G.G. Kuvshinov

Catal. Lett., 70 (2000) pp. 83–91.

Silica aerogels comprising nickel oxide nanoparticles were synthesized with no use of supercritical drying. A high specific surface area (more than 1000 m^2/g), mesoporous structure and considerable stability to sintering up to 900 °C are characteristic of these aerogels. The aerogels were synthesized using the sol-gel method. Filamentous carbon was templated by silica, tetraethoxysilane being used for supplying silica. Carbon was burnt later. Analysis of the aerogel structure revealed the presence of silica nanotubes and nanofibers. Aerogel testing for direct oxidation of H_2S into S^0 demonstrated as high as 60 % conversion of hydrogen sulfide at almost 100 % selectivity under stoichiometric conditions at the temperature range of 300 to 350°C and 73 % conversion at 100 % selectivity at a considerable excess of oxygen at 160°C.

Carbon and Carbon Containing Materials

MODELLING OF THE PROCESSES OF FILAMENTARY CATALYTIC CARBON PRODUCTION FROM METHANE-HYDROGEN MIXTURE IN PERIODIC REACTOR WITH A FLUIDIZED CATALYST BED

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(Novosibirsk, State Technological University, Novosibirsk, Russia)

Scientific Bull. of NSTU, 2 (1999) pp. 127-134.

On the basis of a model of the plug regime reactor with respect to gases and the ideal mixing with respect to catalyst particles, the production of filamentary carbon from a methane-hydrogen mixture was simulated in a periodic reactor with a fluidized catalyst bed. The yield of carbon and time of the catalyst deactivation as the functions of temperature (803-843 K), mixture flow rate (100-140 $m^3/(kg\ h)$, and hydrogen concentration in the mixture (0–30 %) have been calculated.

FORMATION OF FILAMENTOUS CARBON FROM 1,3-BUTADIENE OVER A $NiPd/Al_2O_3$ CATALYST

V.I. Zaikovskii, V.V. Chesnokov, R.A. Buyanov, L.M. Plyasova

Kinetics & Catalysis, 41 (2000) pp. 538-545.

The formation of carbon filaments from 1,3-butadiene over a Ni–Pd/Al_2O_3 catalyst at 400–450 °C was studied by high-resolution electron microscopy and X-ray diffraction analysis. The carbon filaments differ in morphology and in the arrangement of active metal inclusions: (1) abundant ~ 1000 Å thick filaments contain biconical alloy particles in the middle of the filament, (2) thin filaments of a thickness less than 500 Å rolled in helical fashion contain oval-shaped alloy particles in the middle, and (3) in a few filaments that are less than 200 Å thick, alloy particles are positioned at the ends. When the first two types of filaments grow, decomposition of the hydrocarbon occurs at the active sites of the surface with the formation of a carbide microphase with a hexagonal structure. This phase is called the active microphase. When the reaction stops, the active phase decomposes to form carbon and hexagonal nickel. Extensive defects like grain boundaries and stacking fault dislocations are present in the bulk of Ni–Pd alloy particles. The origin of these defects is related to the epitaxial effect of the active microphase particles on the alloy.

SYMMETRIC TWISTED CARBON FILAMENTS FORMED FROM BUTADIENE-1,3 ON Ni–Cu/MgO-CATALYST: GROWTH REGULARITIES AND MECHANISM

V.V. Chesnokov, V.I. Zaikovskii, R.A. Buyanov

J. Molec. Catal. A: Chemical, 158 (2000) pp. 267-270.

High-resolution electron microscopy has been used to study the regularities of formation of symmetric helical carbon filaments from Ni–Cu/MgO-catalyzed butadiene-1,3 decomposition at 450°C. Dissymmetrical spirally twisted carbon filaments have been shown to grow from a single Ni–Cu alloy particle. As the filaments grow, a microphase of metastable nickel carbide Ni_3C forms on the particles' frontal side, whereas the crystal particle of Ni–Cu alloy possesses a series of twinning planes (111) that is parallel to the dissymmetry plane of the crystal and separates the blocks of twins with a face-centered structure. The mechanism of symmetric helical filamentous carbon growth has been suggested.

THE FORMATION OF CARBON FILAMENTS UPON DECOMPOSITION OF HYDROCARBONS CATALYZED BY IRON GROUP METALS AND THEIR ALLOYS

V.V. Chesnokov, R.A. Buyanov

Russ. Chem. Rev., 69 (2000) pp. 623-638.

The structure of filamentous carbon formed upon catalytic decomposition of hydrocarbons of iron group metals and their alloys is considered. The regularities of the deposition of carbon on these metals are generalised. The carbide cycle mechanism of carbon formation is considered in detail. The growth models of some morphological modifications of filamentous carbon are discussed. The bibliography includes 151 references.

ON THE CARBON SOLUBILITY IN THE METALS OF THE IRON GROUP

R.A. Buyanov

Chemistry for Sust. Devel., 8 (2000) pp. 347-352.

The conditions of formation of supersaturated solutions of carbon in the metals of iron group, the influence of supersaturation on their properties and carbon diffusion through metal particles upon hydrocarbon decomposition are considered.

The possibility of transient existence of such systems in metastable state and of their practical application for development of novel synthesis methods is shown.

EFFECT OF MICROSTRUCTURE ON THE OXIDATION RESISTANCE OF POROUS CARBON MATERIALS IN AIR

V.A. Semikolenov, G.S. Litvak, G.V. Plaksin

Inorg. Mater., 36 (2000) pp. 591-594.

The oxidation resistance of porous carbon materials in air was studied by thermal analysis. The effects that the size, ordering, and orientation of carbon microcrystallites and the curvature of the surface of primary particles have on the temperatures of oxidation onset and peak weight loss were examined. The extent and orientation of surface graphite-like layers were shown to have a crucial effect on the oxidation resistance of porous carbon materials, which may remain stable to oxidation up to 700°C, the oxidation temperature of graphite.

KINETICS OF THE GRAPHITIZATION OF DISPERSED DIAMONDS AT "LOW" TEMPERATURES

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J. Appl. Phys., 88 (2000) pp. 4380-4388.

The bulk density graphitized ultra dispersed diamond (UDD) was measured by a gamma-ray attenuation method at 1370-1870 K. These data combined with small angle X-ray scattering (SAXS) and true density measurements of the samples heated at various fixed temperatures were used to study the graphitization kinetics of the UDD. The reaction rate was modeled as a migration rate of the interface between the developing graphite-like carbon and the remaining diamond phase. A "reducing sphere" model was used to obtain the rates from the changes in densities. The estimated kinetic parameters in an Arrhenius expression, namely, the activation energy, E=45±4 kcal/mol, and the pre-exponential factor, A=74±5 nm/s, allow quantitative calculations of the diamond graphitization rates in and around the indicated temperature range. The calculated graphitization rates agree well with the graphitization rates of diamonds with different dispersity estimated from high resolution transmission electron microscopy (HRTEM) data. The large difference between the rates and the kinetic parameters obtained in this study and those estimated by Davies and Evans for the temperature range 2150-2300 K indicates that there are different graphitization mechanisms operating in the "low" and "high" temperature regions.

IN SITU RAMAN INVESTIGATIONS OF SINGLE-WALL CARBON NANOTUBES PRESSURED IN DIAMOND ANVIL CELL

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Aip Conf. Proceedings, 486 (1999) pp. 333-337.

The Raman spectra of single-wall C nanotubes under the pressure up to 10 GPa were measured *in situ* in diamond anvil cell. The breathing mode was clearly seen at pressures < 2 GPa and disappeared at higher pressures. The splitting of TO mode was kept at all steps of pressurizing. This mode shifted from the position 1592 cm^{-1} (at ambient pressure) toward high frequencies almost linearly with the pressure. The shift rate (4.9 cm^{-1}/GPa) appeared to be very close to that of graphite. The irreversible broadening and overlapping of the split components of TO mode at pressures > 2.5. GPa were observed. A possible mechanism of the tube structure transformation under the pressure is discussed.

THIN FILM COLD CATHODE FROM NANOSTRUCTURED CARBON

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V.L. Kuznetsov, A.L. Chuvilin (*Moscow
Lomonosov State University, Moscow, Russia)

AIP Conf. Proceedings, 486 (1999) pp. 444-447.

Thin films of nanostructured carbon material were grown on silicon substrates by a d.c. discharge plasma CVD technique. HREM investigations have shown that the films contain carbon nanotubes and flaked graphite nanocrystallites with predominant orientation of nanotube axes and basal graphene planes of crystallites along a normal to substrate surface. Electron field emission was observed at av. fields above 1 V/mm with emission site d. higher than 106 l/cm^2 and emission c.d. up to 10 mA/cm^2 at 4 V/mm. The prototypes of cathodoluminescent light emitting devices were manufactured with use of the nanostructured carbon films as cold cathodes. A brightness of 1000 cd/m^2 was achieved at operational voltage of about 250 V.

ALIGNED CARBON NANOTUBE FILMS FOR COLD CATHODE APPLICATIONS

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Russia; **Natural Sciences Center of General Physics
Institute, Moscow, Russia)

J. Vac. Sci. Technol. B, 18 (2000) pp. 1059-1063.

Thin film material of oriented multiwall carbon nanotubes was obtained by noncatalytical chemical vapor deposition in a glow-discharge plasma. The film phase components, surface morphology, and structural features were studied by Raman and electron microscopy techniques. Low-voltage electron field emission of thin film nanotube material was obtained and examined in diode configuration. The I-V curves in Fowler-Nordheim coordinates were linear and the corresponding threshold av. field was about 1.5 V/mm. The emission c.d. was up to 50 mA/cm^2 at the field of 5 V/mm. The emission site d. reached 107 cm^{-2} at the same value of electric field.

FORMATION OF C_1-C_5 HYDROCARBONS FROM CCl_4 IN THE PRESENCE OF CARBON-SUPPORTED PALLADIUM CATALYSTS

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I.V. Stoyanova, V.V. Lunin* (*Moscow Lomonosov
State University, Moscow, Russia)

Kinetics & Catalysis, 41 (2000) pp. 776-781.

Along with hydrodechlorination, the formation of C_1 and higher hydrocarbons takes place in a flow system in the presence of catalysts containing 0.5-5.0% Pd supported on a Sibunit carbon carrier at 150-230°C. In the entire range of conditions examined, the reaction products are primarily methane, C_2–C_4 hydrocarbon fractions, and C_5 traces. The catalysts are stable in operation, and a high conversion of CCl_4 was retained for a long time interval. The nonselective formation of linear and branched hydrocarbons is indicative of a radical mechanism of the process.

CARBON SORBENTS FROM THE CEDAR NUTSHELL

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V.K. Duplyakin, B.N. Kuznetsov*,
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Chemistry for Sust. Development, 8 (2000)
pp. 715-721.

The influence of operating parameters of the process of thermal treatment on the texture of carbon sorbents produced by carbonization and activation of cedar nutshell was studied. Data on the molecular sieve structure of cedar-based carbon materials were obtained. Properties of these materials were found to resemble those of industrial carbon sorbents synthesized from coconut shell used for air separation (O_2 – N_2 separation).

Correlation between the yield of porous carbon materials and conditions of activation of carbonized cedar nutshell was established. The activating agent composition, which was optimal in terms of the yield and textural characteristics of the carbon products, was shown to be as follows: 25–80% of steam and 0 - 2% of oxygen. A developed system of micro- and mesopores was characteristic of active carbons synthesized under these conditions.

ON THE METAL BLOCKING IN MICROPORES OF CARBON SUPPORTS

L.B. Okhlopkova, A.S. Lisitsyn, H.P. Boehm*, V.A. Likholobov (*University of Munich, Munich, Germany)

React. Kinet. & Catal. Lett., 71 (2000) pp. 165-171.

Platinum catalysts prepared on activated carbon supports of different origin are compared in the hydrogenation of cyclohexene and cyclooctene, which differ much in their reactivity. A decrease in catalytic activity upon decreasing the dimensions of the micropores in the support and the size of the supported metal particles has been confirmed. The results give evidence against a trivial role of the diffusional factor in such an effect and indicate complete blocking of part of the metal surface in narrow pores.

PALLADIUM CATALYSTS ON ACTIVATED CARBON SUPPORTS. INFLUENCE OF REDUCTION TEMPERATURE, ORIGIN OF THE SUPPORT AND PRETREATMENTS OF THE CARBON SURFACE

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Carbon, 38 (2000) pp. 1241-1255.

A number of activated carbons produced from peat, coconut shell, and by pyrolysis of hydrocarbons have been subjected to treatment with oxygen, hydrogen or ammonia at elevated temperatures to get a representative series of catalyst supports differing in porous structure and surface chemistry (characterized by nitrogen absorption and selective titrations). Palladium was deposited from anionic (H_2PdCl_4), neutral ($Pd(Oac)_2$, in acetone), and cationic ($[Pd(NH_3)_4](NO_3)_2$) complexes. Temperature-programmed reduction, CO chemisorption, and testing in olefin hydrogenation were used to study the possible effects of preparation variables. The origin of the carbon support and the temperature of the catalyst reduction with hydrogen proved to have a profound influence on the properties of the catalysts. In contrast, no unambiguous correlation has been found between catalyst properties and the pretreatments of the carbons. It is concluded that the effect of the support comes mainly from the differences in the porous structure of the carbons, and occurrence of steric hindrance for organic substrates in contacting the metal particles on the microporous supports is suggested.

PROPERTIES OF Pt/C AND Pd/C CATALYSTS PREPARED BY REDUCTION WITH HYDROGEN OF ADSORBED METAL CHLORIDES. INFLUENCE OF PORE STRUCTURE OF THE SUPPORT

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Appl. Catal. A: General, 204 (2000) pp. 229-240.

A number of catalysts have been prepared by adsorption of H_2PdCl_4 and H_2PtCl_6 on activated carbon of different origin followed by drying and reduction in flowing hydrogen. They were characterized by CO chemisorption and by liquid-phase hydrogenation of cyclohexene, cyclooctene and nitrobenzene. A decisive influence of the pore structure of the support on the catalyst properties has been found. By a proper choice of the preparation conditions, it proved possible to obtain a sufficiently high dispersion of the supported metal on an any one of the activated carbon used. However, catalytic activity per mass of metal reached a maximum in the range of intermediate metal dispersion in narrow pores of the supports, which renders part of the metal surface inaccessible to the organic substrates. Such a blocking effect proved especially significant for Pt catalysts on the activated carbons with the smallest micropores.

STUDY OF MULTIWALLED GRAPHITE NANOTUBES AND FILAMENTS FORMATION FROM CARBONIZED PRODUCTS OF POLYVINYL ALCOHOL VIA CATALYTIC GRAPHITIZATION AT 600-800^{0}C IN NITROGEN ATMOSPHERE

O.P. Krivoruchko, N.I. Maksimova, V.I. Zaikovskii, A.N. Salanov

Carbon, 38 (2000) pp. 1075-1082.

The catalytic graphitization of amorphous carbon matrix was carried out at the temperature range of 600-800^{o}C in nitrogen atmosphere. Amorphous carbon matrix with uniformly distributed Fe particles was obtained via catalytic carbonization of polyvinyl alcohol (PVA) at temperatures up to 600^{o}C in nitrogen atmosphere. Using transmission electron microscopy (TEM), selected area diffraction (SAD), scanning electron microscopy (SEM), and X-ray diffractometry

(XRD), graphite structures of three types were found in products of catalytic graphitization of amorphous carbon matrix: multiwalled graphite shells wrapping the catalyst particles, cockle-shelled graphite filaments (CSF), and multiwalled graphite nanotubes (MWNT). It is supposed that the formation of CSF proceeds through the dissolution of amorphous carbon in the metal, transformation of the catalyst particles into a liquid state and transfer of dissolved carbon via intermediates to growing filaments. Graphite nanotubes nucleate at the matrix surface and then grow in the porous space of the matrix.

CATALYTIC SYNTHESIS OF CARBON NANOSTRUCTURES FROM POLYMER PRECURSORS

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J. Molec. Catal. A: Chemical, 158 (2000) pp. 301-307.

Carbon nanostructures were prepared by decomposition of polyethylene and polyvinyl alcohol using an iron catalyst at 600-750°C under a nitrogen flow. Heating a uniform distribution of catalyst particles in the polymer bulk to 600°C under flowing nitrogen led to the formation of amorphous carbon incorporating uniformly distributed catalyst particles. Subsequent heating of the samples to 750°C in a nitrogen flow led to the catalytic graphitization of the amorphous carbon matrix with the formation of different carbon nanostructures, i.e. carbon nanotubes. The mechanism of the formation of the obtained carbon nanostructures is discussed.

RHEOLOGICAL PROPERTIES OF PLASTIC CARBON COMPOSITES

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Chem. for Sustainable Devel., 8 (2000) pp. 667-674.

Performance of catalytic processes is to a large extent determined by the shape and size of the catalyst grains. For each catalytic process, the shape and size can be chosen depending on the process conditions, kinetic regularities and specific catalyst activity in order to provide the maximal rate and optimal hydrodynamic parameters of the process. Existent commercial carbon supports are conventionally produced as granules simplest in shape. Fabrication of grains and products of complex shape faces a number of difficulties due to specific rheological behavior of plastic slurries. Therefore, the chemical composition and rheological characteristics of carbon slurries must be optimized. Rheological properties of plastic carbon mixtures are studied using water, aqueous dispersions and aqueous solutions of polymers as disperse media. The flow mode of carbon black dispersions is shown to change from pseudoplastic to dilatational depending on the nature of the disperse medium. Concentration dependencies are obtained for spring and elasticity moduli. The spring modulus of a technical carbon – polymer solution mixture is shown practically not to change with an increase in the polymer content in the slurry but the elasticity modulus to be several times decreased. The results obtained are used to develop the technology for manufacturing of molded carbon products of different shapes, including honeycomb structures.

FLUORINATED CAGE MULTIWALL CARBON NANOPARTICLES

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Chem. Phys. Lett., 322 (2000) pp. 231-236.

Multiwall carbon nanoparticles from the inner part of a deposite grown onto a cathode in an arc-discharge condition were fluorinated at room temperature using volatile fluoride BF_3. The sample produced was characterized by means of X-ray diffraction (XRD), infrared (IR) and X-ray photoelectron spectroscopy (XPS). These methods point to the presence of covalent C-F bonds in the sample with retention of the sp^2-hybridizited carbon atoms composing the cage tubular or quasi-spherical shells. Transmission electron microscopy (TEM) indicated a decrease of cage nanoparticles in the fluorinated material relative to the pristine sample that may be connected with unrolling the nanotubes during fluorination.

INVESTIGATION OF VARIOUS CARBON MODIFICATIONS BY MEANS OF RAMAN SPECTROSCOPY

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Chem. for Sustainable Devel., 8 (2000) pp. 43-47.

The investigation of natural substances with a high carbon content (CS), as well as natural and synthetic crystal modifications of carbon including diamonds, graphites, fullerenes, has been carried out by means of Raman light scattering. It has been shown that the major constituent of CS is graphite with various ordering degree. Along with crystal graphite phase (sp^2 hybridization of carbon), ultrafine graphite is also present, as well as the amorphous phase with the elements of sp^2 hybridization of carbon. The possibility to use the parameters of Raman spectra of impact diamonds as a type-morphous index is demonstrated with the samples from Popigay and Karsk astroblemes as an example.

CARBON DISPERSION AND MORPHOLOGY IN CARBON-MINERAL ADSORBENTS

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J. Colloid Interf. Sci., 229 (2000) pp. 431-439.

Carbon-mineral composite adsorbents prepared by deposition of carbon on various mineral supports have been studied extensively by a new textural approach. The evidence of significant influence of both organization of initial mineral support porous space and mobility of carbon precursors over the surface of mineral support on carbon localization has been obtained. Restricted mobility of carbon precursors leads to homogeneous distribution of carbon clusters over the support surface despite the presence of narrow mesopores in the structure of the support if the entire support surface is equiaccessible. Unrestricted mobility over the smooth surface of the mineral support without narrow mesopores leads to the similar resulting carbon distribution. However, unrestricted mobility of carbon precursors in densely packed porous materials seems to be the reason for carbon pulling and deposition in narrow mesopores. These peculiarities of carbon deposition influence the carbon/mineral (hydrophobic/hydrophilic) composition of the composite surface. Trapping of carbon in narrow mesopores leads to a decrease and, in contrast, homogeneous dispersion of carbon over the whole support surface leads to an increase in the part of the composite surface, which can be appropriated to carbon.

Reactions over Pt-Group Metals

REACTION OF NH_2 SPECIES WITH HYDROGEN AND NO ON THE Pt(100)-1×1 SURFACE

M.Yu. Smirnov, D.Yu. Zemlyanov

J. Phys. Chem. B, 104 (2000) pp. 4661-4666.

The formation of the $NH_{2,ads}$ amino species and its further reaction with hydrogen and NO on the unreconstructed Pt(100) surface were studied by means of high-resolution electron energy loss spectroscopy (HREELS) and temperature-programmed reaction (TPR) spectroscopy. The $NH_{2,ads}$ amino species forms during the reaction between H_{ads} and NO at 300 K. $NH_{2,ads}$ can be oxidized by NO at a temperature higher than 260 K. The reaction at $T \geq 300$ K results in the evolution of N_2 and water. An essential amount of N_{ads} accumulates on the surface after the reaction at ~260 K and desorbs as a low-temperature TPR peak of N_2 at 320 K. TPR in a saturated coadsorption layer of NO_{ads} and $NH_{2,ads}$ prepared at 100 K shows an "explosive" behavior, manifesting itself in the evolution of narrow TPR peaks of N_2 and H_2O at ~370 K. TPR in an unsaturated coadsorption layer of NO_{ads} and $NH_{2,ads}$ proceeds at a much lower temperature of <300 K, resulting in the "nonexplosive" desorption peaks of N_2 and H_2O. The reaction between the $NH_{2,ads}$ and H_{ads} species in the temperature range of 350-470 K results in ammonia evolution. At T<400 K, NH_3 forms through the addition of a hydrogen atom to $NH_{2,ads}$ and competes with the H_{ads} recombination. At higher temperature, > 400 K, the dissociation of $NH_{2,ads}$ serves as a source of hydrogen atoms for the $NH_{2,ads}$ hydrogenation, leading to the parallel evolution of ammonia along with N_2 and H_2. The mechanism of the formation of $NH_{2,ads}$ species and its further reaction with NO and hydrogen on the Pt(100)-(1x1) surface are discussed in detail.

NO AND DEUTERIUM CO-ADSORPTION ON THE RECONSTRUCTED Pt(100)-*hex* SURFACE: A TEMPERATURE PROGRAMMED REACTION STUDY

E.I. Vovk, M.Yu. Smirnov, D.Yu. Zemlyanov

Surf. Sci., 453 (2000) pp. 103-111.

The deuterium adsorption at 270 K on a reconstructed Pt(100)-*hex* surface covered by NO_{ads} was studied by means of temperature programmed reaction (TPR). In the case of adsorption on a clean

Pt(100)-*hex* surface the saturated D_{ads} coverage is 0.06 ML at $P_{H2}=6x10^{-8}$ mbar, whereas the D_{ads} uptake is enhanced considerably by NO pre-adsorption. First the D_{ads} uptake increases with increasing NO_{ads} coverage, θ_{NO}, reaching a maximum at $\theta_{NO} \approx 0.25$ ML, and then decreases to zero. This phenomenon is explained as follows. The NO adsorption on the *hex* surface leads to the formation of 1x1 islands saturated by NO_{ads} and surrounded by the *hex* phase. The NO_{ads}/1x1 islands are assumed to modify the *hex* phase adjacent to the island boundaries, adapting this area for deuterium adsorption.

TPR in the co-adsorption layer of NO_{ads} and D_{ads} is initiated by D_2 desorption and shows an 'explosive' behaviour, manifesting itself in the narrow TPR peaks of N_2 and D_2O at ~370 K. The NO_{ads} pre-coverage affects the reaction temperature as well. Thus, at NO_{ads} coverage of 0.35-0.40 ML the temperature of the surface explosion increases abruptly by ~15-20 K. At this coverage the NO_{ads}/1x1 islands are supposed to modify the rest of the hex phase so that, after further D_2 adsorption, the surface becomes completely saturated by D_{ads} and NO_{ads} species. A possible mechanism for this is discussed.

EFFECT OF NO ON D_2 ADSORPTION ON THE Pt(100)-(*hex*) SURFACE

E.I. Vovk, M.Yu. Smirnov, D.Yu. Zemlyanov

J. Molec. Catal. A: Chemical, 158 (2000) pp. 395-398.

The influence of NO on the desorption of D_2 on the Pt(100)-(hex) surface was studied by means of temperature-programmed reaction (TPR). Deuterium adsorbs negligibly on Pt(100)-(hex) at T=270 K, whereas an addition of a small amount of NO to D_2 increases drastically the adsorption capacity of Pt(100)-(hex) towards deuterium. The same phenomenon was observed on the surface pre-covered with NO_{ads} as well. As the NO_{ads} pre-coverage increases, the uptake of D_2 first increases, then reaches a maximum at $\theta_{NO} \approx 0.25$ ML, and finally falls down to zero for the NO_{ads} saturated layer.

The following explanation is supposed. Upon adsorption on the Pt(100)-(hex) surface, NO lifts the (hex) reconstruction and forms the dense NO_{ads}/1x1 islands surrounded by the clean (hex) surface. A limited area of the (hex) phase, which is immediately adjacent to the boundaries of the NO_{ads}/1x1 islands, is supposed to be distorted and could be able to absorb deuterium.

NON-LINEAR PROCESSES ON Pt, Pd, Rh, Ir AND Ru SURFACES IN THE NO-HYDROGEN REACTION

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J. Molec. Catal. A: Chemical, 158 (2000) pp. 115-128.

The present paper reviews research in the field of $NO+H_2$ reactions over Pt, Rh, Pd, Ir and Ru surfaces. Emphasis is placed on the ability of these platinum group metals to produce oscillations in both reaction rate and selectivity, in addition to other non-linear processes such as hysteresis phenomena. In the case of Rh, non-linearity is related to periodic transitions between N- and O-rich surfaces, with O destabilising the N-adlayer and causing an acceleration in the N_2 production. However, in the case of Pt, the important step involves the creation of vacant sites required for NO dissociation, whereby products leaving the surface facilitate an autocatalytic rise in the concentration of such vacancies, and, hence, reaction rate. Ir positions itself between the former two, because oscillations have been observed in two different regimes. Such a lower-temperature Pt-like and higher-temperature Rh-like behaviours have been observed on different IR surfaces. New results gained from field emission microscopy (FEM) and field ion microscopy (FIM) measurements are presented to consolidate the lower-temperature Pt-like behaviour, and confirm the dualistic nature of Ir. No oscillations in rate have been observed over Pd(111) or Ru(0001). The Ru surface exhibits selectivity to N_2 of almost 100% even in large excess of hydrogen.

STUDY OF H_2, O_2, CO ADSORPTION AND CO+O_2 REACTION ON Pt(100), Pd(110) MONOCRYSTAL SURFACES

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J. Molec. Catal. A: Chemical, 158 (2000) pp. 155-160.

Nanoscale changes in the surface morphology of Pd particles that accompany the uptake of hydrogen have been studied *in situ* by Field Electron Microscopy (FEM). Exposure of a Pd tip to H_2 at low temperatures led to the formation of extruding PdH_x particles on top of the Pd tip. Growth of these particles proceeds in a "staccato" manner. When most of the hydrogen have been removed from the sample by heating in vacuum, Pd crystallites remain on the surface. They are quite stable up to about 700 K, where they melt back into the bulk of the tip. A sharp low temperature H_2-peak (220 K) appears in the TD spectra as a result of decomposition of PdH_x hydrides on Pd(110) single crystal surface. During the O_2+H_{ads} reaction, a hydrogen-modified Pt(100)-(hex) surface shows an increase in the population of atomic oxygen states: three O_{ads} states are observed by high resolution electron energy loss spectroscopy (HREELS) as a result of the presence of defect sites. The reactivity of these new oxygen states to CO has been investigated with thermal decomposition spectroscopy (TDS).

Catalysis by Sulfides

AN *AB INITIO* MOLECULAR ORBITAL STUDY OF THE HYDROGEN SORBED SITE IN Co/MoS$_2$ CATALYST

I.I. Zakharov, **A.N. Startsev**

J. Phys. Chem. B, 104 (2000) pp. 9025-9028.

A cluster model quantum chemical approach is used to study the electronic structure of Co in bimetallic sulfide catalysts Co/MoS_2. The oxidative addition of hydrogen to the Co-Mo component is considered. *Ab initio* HF/MP2 and DFT calculations show that hydrogen occluded in the catalyst bulk is sorbed on the cobalt ion, and stabilizes the (d^6) electronic state of cobalt ions in the sulfide catalysts. This electronic state is rather active, when surface sites interact with the S-containing reagents participating in the HDS catalysis. A model of active sites on the Co/MoS_2 catalyst is used to discuss the suggested molecular mechanism of the HDS catalysis.

CONCERTED MECHANISMS IN HETEROGENEOUS CATALYSIS BY SULFIDES

A.N. Startsev

J. Molec. Catal. A: Chemical, 152 (2000) pp. 1-13.

This paper summarizes some new evidences of the possibility of concerted mechanisms in the heterogeneous catalysis by sulfides. Several aspects are discussed: main regularities of thiophene and THT hydrogenolysis mediated by the well-characterized sulfide catalysts of different composition; electronic structure of the metals entering into the composition of the active component of both bulk and supported sulfide catalysts; mechanism of the active Ni(Co) metals and occlusion of hydrogen atoms into the MoS_2 matrix; mechanism of the homolytic hydrogen adsorption on the sulfide hydrotreating catalysts; synchronous interaction of the reactive molecules in the coordination sphere of the bimetallic active centers – proton and electron transfer; use of the energy released during exothermic reaction steps in the catalytic cycle. Catalytic transformations over the sulfide HDS catalysts are considered to belong to the acid-base catalysis. The profound identity of the mechanisms of heterogeneous, homogeneous and enzyme catalysis is discussed.

OXIDATIVE ADDITION OF DIHYDROGEN TO THE BIMETALLIC SULFIDE CATALYSTS: EVIDENCES BY X-RAY PHOTOELECTRON SPECTROSCOPY

A.N. Startsev, A.V. Kalinkin, I.I. Zakharov,
D.G. Aksenov, V.N. Parmon

J. Molec. Catal. A: Chemical, 151 (2000) pp. 171-177.

Reversible transformations Ni(IV)⇔Ni(II) in the alumina and Sibunit supported (Ni,Mo) sulfide catalysts were observed after *in situ* thermal treatment of catalysts in a X-ray photoelectron spectrometer chamber. The phenomenon is interpreted as a reductive elimination of occluded hydrogen under low pressure and high temperature, and oxidative addition of hydrogen after catalyst treatment with a (H_2+H_2S) mixture.

Copper-Containing Oxide Catalysts

MODERATE-TEMPERATURE REDUCTION OF COPPER CHROMITE BY HYDROGEN AND HYDROGEN DESORPTION FROM THE SURFACE OF REDUCED CHROMITE

A.V. Khasin, I.I. Simentsova, T.M. Yurieva

Kinetics & Catalysis, 41 (2000) pp. 282-286.

The reduction of copper chromite $CuCr_2O_4$ by hydrogen at 300–573 K and a hydrogen pressure of 4×10^4-8×10^4 Pa and hydrogen desorption from the surface of a reduced sample are studied. The rate of copper chromite reduction becomes high at temperatures above 473 K. Hydrogen desorbs from the surface of metallic copper covering the surface of chromite during its reduction. The heat of hydrogen adsorption on the metallic copper is almost independent of the surface coverage, 70–80 kJ/mol.

STRUCTURE TRANSFORMATIONS OF COPPER CHROMITE UNDER REDUCTION-REOXIDATION CONDITIONS

L.M. Plyasova, **I.Yu. Molina**, **T.A. Krieger**,
L.P. Davydova, T.M. Yurieva

J. Molec. Catal. A: Chemical, 158 (2000) pp. 331-336.

Structure transformations accompanying reoxidation preliminary reduced at 270°C copper chromite were studied using X-ray powder diffraction method, and comparison of the structures of the initial and reoxidized copper chromite was carried out. It is shown that the reoxidized spinel is non-stoichiometric and possibly contains some amount of hydrogen in the form of protons bonded to the lattice oxygen. Differences of reversible phase transformation of copper chromite under reduction-reoxidation conditions from reversible polymorphysm of copper chromite with temperature variations are analyzed.

ROLE OF THE Cu-Co ALLOY AND Co-CARBIDE IN HIGHER ALCOHOL SYNTHESIS

G.G. Volkova, T.M. Yurieva, L.M. Plyasova,
M.I. Naumova, V.I. Zaikovskii

J. Molec. Catal. A: Chemical, 158 (2000) pp. 389-393.

Formation and decomposition of the Cu-Co alloy and Co_2C were studied using *in situ* X-ray diffraction (XRD), TG-DTA and TEM techniques. Cu-Co alloy with ratio Cu:Co = 1:1 has been obtained under treatment of $CuCoO_2$ with hydrogen at 230-300^{0}C. Co_2C was formed from Cu-Co alloy at 280-310^{0}C and decomposed at 390-400^{0}C under CO. It was shown that the role of Cu-Co alloy consisted in formation of cobalt carbide was able to activate CO undissociatively that led to oxygenates synthesis.

DYNAMICS OF STRUCTURAL TRANSFORMATIONS IN THE REDUCTION OF COPPER ALUMINATE

L.M. Plyasova, T.M. Yurieva, I.Yu. Molina,
T.A. Krieger, A.M. Balagurov*, L.P. Davydova,
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Kinetics & Catalysis, 41 (2000) pp. 429-436.

The dynamics of structural transformations during copper aluminate reduction in the temperature range used for catalyst activation was studied by high-temperature X-ray analysis under controlled conditions (hydrogen, 20–400°C). The techniques of neutron diffraction analysis, IR spectroscopy, chemical phase analysis, and electron microscopy were also used at particular stages. In the course of reduction, copper metal is deposited onto the surface of spinel crystals from the bulk. Spinel becomes cation-deficient with respect to copper. An analysis of powder diffraction patterns demonstrated that copper is reduced and released from tetrahedral positions of the spinel structure at temperatures below ~300°C and from octahedral positions only at temperatures above 300°C. In this case, a redistribution of aluminum ions was observed simultaneously. It is likely that the electrical neutrality is attained by the formation of OH groups, the appearance of which in reduced samples was detected by IR spectroscopy and confirmed by neutron diffraction analysis. At a reduction temperature of 400°C, the oxygen framework was partially disintegrated. The structures of reduced copper aluminates and chromites were compared.

Catalysis by Metal Complexes

TRANSFORMATIONS IN THE Pt(IV) COMPLEX CONTAINING *N*-NITROSATED ETHYLENEDIAMINE IN A HYDROCHLORIC ACID MEDIUM: CRYSTAL AND MOLECULAR STRUCTURE OF *trans**-[Pt($H_2NCH_2CH_2NNO{\cdot}H$)$NO_2Cl(NH_3Cl)$*]Cl

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Russ. J. Inorg. Chem., 45 (2000) pp. 344-353.

The transformations of the N-nitrosated complex *trans**-[Pt($H_2NCH_2CH_2NNO$)$NO_2Cl(NH_3Cl)$*] in a hydrochloric acid medium are studied. Reaction products depend on reaction conditions (temperature, duration): the *N*-nitrosated ethylenediamine ligand can either be protonated to form *trans**-[Pt($H_2NCH_2CH_2NNO$ H)$NO_2Cl(NH_3Cl)$*]Cl, be *N*-denitrosated to produce the initial triamine complex *trans**-[Pt($H_2NCH_2CH_2NH_2$)$NO_2Cl(NH_3Cl)$*]Cl, or be involved in the redox reaction to convert into the chloramine ligand $H_2NCH_2CH_2NHCl$, which then loses chlorine and converts into ethylenediamine. The isolated compounds are characterized by elemental analyses, IR spectroscopy, and ^{195}Pt and ^{14}N NMR. The protonated complex *trans**-[Pt($H_2NCH_2CH_2NNO$ H)$NO_2Cl(NH_3Cl)$*]Cl is studied by X-ray crystallography for the first time. Crystals are orthorhombic: $a = 9.748(2)$ Å, $b = 12.534(3)$ Å, $c = 9.026(2)$ Å, Z = 4, space group $Pna2_1$, $V = 1102.8(4)$ Å3, $\rho_{calc} = 2.732$ g/cm^3, $\mu(MoK_\alpha) = 13.442$ mm^{-1}, $F(000) = 840$, M = 453.59. The proton, whose coordinates are found experimentally, is attached to the oxygen of the nitroso group.

PREPARATION OF POLYOXOMETALATE-STABILIZED COLLOIDAL SOLUTIONS OF PALLADIUM METAL AND CATALYSTS SUPPORTED ON THEM

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Kinetics & Catalysis, 41 (2000) pp. 844-852.

Sols containing Pd(0) clusters with polyoxo anions are prepared by the reduction of colloidal solutions of polyhydroxo complexes of Pd(II) in the presence of Mo(VI), W(VI), V(V), and Nb(V) polyoxo anions. The cluster sizes varied within the limits of 1–10 nm depending on the nature of the polyoxo anion. The stability of sols toward coagulation depends on the ratio between the palladium and polyoxo anion amounts in solution and on the composition of the solvent. Supported Pd catalysts are obtained by the adsorption of particles from sols; Pd can exist in these catalysts as individual particles or associates or form filamentary structures.

FORMATION OF HETEROMETAL RUTHENIUM COMPLEXES WITH NONFERROUS METALS IN NITRITE SYSTEMS

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Russ. J. Inorg. Chem., 45 (2000) pp. 728-733.

The fact of interaction of ruthenium nitrite complexes with copper(II) and nickel(II) salts in aqueous solutions was established by NMR, EPR, and electronic spectroscopy. The formation of heterometal complexes was assumed. This accounts for the fact that ruthenium is accompanied by these metals during refinement according to the nitrite technology**.**

ORTHO-METALATED COMPLEXES OF 2,6-DIPHENYLPYRIMIDIN-4-ONE

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Russ. J. Inorg. Chem., 45 (2000) pp. 1574-1580.

The palladium(II) and platinum(II) *ortho*-metalated complexes of 2,6-diphenylpyrimidin-2-one (LH_2), [Pd(LH)Cl] and [MLEn] (M=Pt, Pd), and of 2-(*ortho*-bromophenyl)-6-phenyl-5-bromopyrimidin-4-one (LBr_2) are synthesized with the use of the *ortho*-palladized complex [Pd(LH)Cl] as a selective reagent. The structures of the compounds are studied by one- and two-dimensional (homonuclear and heteronuclear) ^{1}H and ^{13}C NMR spectroscopy.

HOMOPOLYMERIZATION OF 4-METHYL-1-PENTENE AND ITS COPOLYMERIZATION WITH ETHYLENE IN THE PRESENCE OF ZIRCONOCENE CATALYSTS

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Polymer Sci., Ser. A, 42 (2000) pp. 126-131.

Homopolymerization of 4-methyl-1-pentene and its copolymerization with ethylene in the presence of catalysts based on zirconocenes, $[(CH_3)_5Cp]ZrCl_3$, $[(CH_3)_2C(Cp)_2]ZrCl_2$, $[(CH_3)_2C(Ind)_2]ZrCl_2$, $[(C_6H_5)(C_2H_5)C(Ind)_2]ZrCl_2$, $[(CH_3)_2Si(Ind)_2]ZrCl_2$, $[(CH_3)_2C(CH_3Cp)(Flu)]ZrCl_2$, and $[(Ph)_2C(Cp)(Flu)]]ZrCl_2$, were studied. It was shown that the order of loading of the reagents affects the yield of poly(4-methyl-1-pentene). Unsymmetrical, bridged metallocenes exhibit the highest activity in polymerization. For the $[(CH_3)_2C(CH_3Cp)(Flu)]ZrCl_2$–methylaluminoxane system, formation of a syndiotactic poly(4-methyl-1-pentene) was observed. In the copolymerization of 4-methyl-1-pentene with ethylene, conditions providing preparation of a linear LDPE with a variable content of 4-methyl-1-pentene units were determined. The effect of the molar ratio of methylaluminoxane: Zr on the yield and composition of the resulting copolymer was revealed.

POLYMERIZATION AND COPOLYMERIZATION OF ETHYLENE WITH HIGHER α-OLEFINS USING METALLOCENE CATALYSTS WITH INDENYL LIGANDS

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Polymer Sci., Ser. A, 42 (2000) pp. 1298-1303.

The kinetics of the polymerization and copolymerization of ethylene with 1-octene and 4-methyl-1-pentene initiated by five bis(indenyl) derivatives of metallocene catalysts differing by chirality and substituents in bridge groups was studied. The activity of the catalysts was found to depend on their structure and the temperature of polymerization. It was shown that high-molecular-mass polymers may be prepared with a high yield at temperatures suitable from the technological viewpoint (70–80°C). The thermal characteristics of the resulting polymers were determined by DSC.

KINETICS AND MECHANISM OF WATER CATALYTIC OXIDATION BY A $Ru^{3+}(bpy)_3$ COMPLEX IN THE PRESENCE OF COLLOIDAL COBALT HYDROXIDE

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Kinetics & Catalysis, 41 (2000) pp. 340-348.

Kinetics of the catalytic oxidation of water to molecular oxygen by a tris(bipyridyl) Ru(III) complex is studied in the presence of colloidal cobalt hydroxide stabilized by starch. Oxidant consumption follows the first-order rate law with respect to the oxidant concentration. The dependence of the apparent rate constant of this process on the catalyst concentration, initial oxidant concentration, and initial concentration of its reduced form was determined. The dependence of the oxygen yield on H^+ at pH 7–11 and a catalyst concentration of 10^{-7}-10^{-3} mol/l is studied. An intermediate product of the reaction was found, which is probably a bridged peroxo complex of cobalt. The kinetic scheme and mechanism of the reaction is proposed, which agree with experimental observations.

STABILITY AND REACTIVITY OF LOW-SPIN FERRIC HYDROPEROXO AND ALKYLPEROXO COMPLEXES WITH BIPYRIDINE AND PHENANTROLINE LIGANDS

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J. Molec. Catal. A: Chemical, 159 (2000) pp. 243-245.

In this work the first-order rate constants of self-decomposition of hydroperoxo and alkylperoxo complexes $[Fe(bpy)_2(OOH)Py](NO_3)_2$ (**2a**-Py), $[Fe(phen)_2(OOH)Py](NO_3)_2$ (**2b**-Py) and $[Fe(bpy)_2(OOtBu)CH_3CN](NO_3)_2$ (**3a**-CH_3CN) were determined in the presence of various substrates and at various temperatures. It was observed, that the alkylperoxo species are far less stable than corresponding hydroperoxo intermediates, k=1.2×10^{-2} s^{-1} (**3a**-CH_3CN in CH_3CN at -10°C) and k=2×10^{-4} s^{-1} (**2a**-Py in CH_3CN at -10°C). The sixth ligand (Py in **2a**-Py and **2b**-Py; CH_3CN in **3a**-CH_3CN) can be replaced by other donor molecules B in appropriate solvent systems. Using d_9-*t*BuOOH, ^{2}D NMR signals of *t*BuOO moieties of complexes **3a**-CH_3CN, **3a**-CH_3OH and **3a**-H_2O were observed. The rate of decomposition of hydroperoxo complexes $[Fe(bpy)_2(OOH)B](NO_3)_2$ (**2a**-B), where B are derivatives of Py (3-Br-Py, 3-Me-Py, 4-Me-Py and $4-Me_2N-Py$) increases with the growth of basisity of B (push effect). Such effect is markedly smaller for alkylperoxo species $[Fe(bpy)_2(OO\textit{t}Bu)B](NO_3)_2$ (**3a**-B). The addition of organic substrates (cyclohexane, cyclohexene, methyl phenyl sulfide) in concentrations up to 3 M at -10°C to +20°C does not noticeably change the rate of self-decomposition of **2a**-B, $[Fe(phen)_2(OOH)B](NO_3)_2$ (**2b**-B) and **3a**-B. Thus the intermediates concerned do not directly react with organic substrates. The reactivity patterns of **2a**-B, **2b**-B and **3a**-B were characteristic for free radical oxidation. $OH^{\cdot}$ and $HO_2^{\cdot}$ radicals were trapped in solution containing **2a**-Py, and $\textit{t}BuOO^{\cdot}$ free radicals were detected in solution in the presence of **3a**-B. The determined rates of self-decomposition of complexes **2a**-B, **2b**-B and **3a**-B can be used for evaluation of the upper limit for their reactivity towards organic substrates.

Heteropolycompounds in Catalysis

POTENTIOMETRIC MONITORING OF THE STATE OF HOMOGENEOUS OXIDATION CATALYSTS BASED ON HETEROPOLY ACIDS

E.G. Zhizhina, V.F. Odyakov, K.I. Matveev

Russ. J. Appl. Chem., 73 (2000) pp. 824-827.

Redox potentials *E* and pH values are measured in 0.2 M aqueous solutions of $H_{3+n}PV_nMo_{12-n}O_{40}$ (HPA-n, 2≤n≤4) and products of their reduction by hydrazine-hydrate to $H_{3+n+m}PV^{IV}_{m}V^{V}_{n-m}Mo_{12-n}O_{40}$ (H_mHPA-n, 0≤m≤n). The dependencies *E*=f(m) and pH=φ(m) are offered as calibrating curves for the control of a degree of reduction m (m=$[V^{IV}]/[H_mHPA\text{-}n]$) in processes of oxidation of alkylphenols (2,6-dimethylphenol, 2,6-di-tert-butylphenol, 2-methyl-1-naphthol) in appropriate alkyl-1,4-quinones by HPA-n solutions.

REDOX POTENTIALS OF MOLYBDOVANADOPHOSPHORIC HETEROPOLY ACIDS IN AQUEOUS SOLUTIONS

V.F. Odyakov, E.G. Zhizhina, K.I. Matveev

J. Molec. Catal. A: Chemical, 158 (2000) pp. 453-456.

Redox potentials *E* and pH values were measured in 0.2 and 0.01 M solutions of partly reduced heteropoly acids $H_{3+x+m}PV^{IV}_{m}V^{V}_{x-m}Mo_{12-x}O_{40}$ (H_mHPA-*x*, 1≤*x*≤4, 0≤*m*≤*x*). The potentials were compared to the redox potential of a couple VO_2^+ / VO^{2+} which is in equilibrium with various HPA-x_m anions. It was found that all HPA-x_m anions as VO_2^+ and VO^{2+} cations are one-electron oxidants / reductants.

REDOX POTENTIALS OF MOLYBDOVANADOPHOSPHORIC HETEROPOLY ACIDS IN AQUEOUS SOLUTIONS

V.F. Odyakov, E.G. Zhizhina, K.I. Matveev

Russ. J. Inorg. Chem., 45 (2000) pp. 1258-1266.

The redox potentials (*E*) and the pH values for 0.01–0.2 M solutions of molybdovanadophosphoric heteropoly acids $H_{3\pm n}PV_m{}^{V}Mo_{12-n}O_{40}$ (HPA-*n*, 1≤*n*≤4) and of their reduced forms $H_{3+m+n}PV_m{}^{IV}V_{n-m}{}^{V}Mo_{12-n}O_{40}$ (H_mHPA-*n*, 0≤*m*≤*n*) were measured. The *E* values are determined by the redox potential of the VO_2^+/VO^{2+} pair, which exists in an equilibrium with the heteropoly anions. The equilibrium fraction of the VO^{2+} cation ($\beta_{IV}=[VO^{2+}]_{eq}/[V_\Sigma{}^{IV}]$) detached from the heteropoly anion H_mHPA-*n* is greater than the fraction of the detached VO_2^+ cation ($\beta_V=[VO_2^+]_{eq}/[V_\Sigma{}^{V}]$). The β_{IV}/β_V ratio decreases as *n* increases and passes through a maximum with an increase in *m*. The resulting dependencies were interpreted in terms of the concept that the HPA-*n* and H_mHPA-*n* anions participate in one-electron transfer.

CATALYTIC OXIDATION OF 2,6-DIALKYLPHENOLS BY OXYGEN TO THE CORRESPONDING 2,6-DIALKYL-1,4-BENZOQUINONES IN PRESENCE OF P-Mo-V HETEROPOLY ACIDS

I.G. Kolesnik, E.G. Zhizhina, K.I. Matveev

J. Molec. Catal. A: Chemical, 153 (2000) pp. 147-154.

A new method for obtaining 2,6-dialkyl-1,4-benzoquinones (DAQ) by oxidation of 2,6-dimethyl- and 2,6-ditertbutylphenols (DAP) by molecular oxygen in a two-phase “water-organic” system in the presence of P-Mo-V heteropoly acids and their salts has been proposed. The selectivity of oxidation of DAP to DAQ (that is 75 to 85%) depends both on the nature of the organic solvent (organic phase) and the number of vanadium atoms (**n**) in a HPA-n molecule (1≤**n**≤6) (aqueous phase). As **n** increases, the selectivity towards HPA-n rises essentially. The rate and selectivity of oxidation are strongly dependent on the concentration of AcOH in aqueous phase. The optimal [AcOH] in the catalyst is 10 to 20 vol.% for DMP oxidation and 35 to 40 vol.% for DTP oxidation. Oxidation of DAP to DAQ in the presence of P-Mo-V heteropoly acids is an environmentally friendly process. Investigated catalysts exhibit high stability because their activity and selectivity remain constant.

KINETICS AND MECHANISM OF THIOETHER OXIDATION WITH H_2O_2 IN THE PRESENCE OF Ti(IV)-SUBSTITUTED HETEROPOLYTUNGSTATES

O.A. Kholdeeva, L.A. Kovaleva,
R.I. Maksimovskaya, G.M. Maksimov

J. Molec. Catal. A: *Chemical*, 158 (2000) pp. 223-229.

Kinetics of thioether oxidation with concentrated (86%) and diluted (35%) aqueous H_2O_2 in the presence of catalytic amounts of $(Bu_4N)_7\{[PW_{11}O_{39}Ti]_2OH\}$ dimeric heteropolytungstate (**1**) has been studied in acetonitrile. With 86% H_2O_2 the reaction was found to be first order in the oxidant, 0.5 order in the catalyst and practically independent on the sulfide concentration and its nature, whereas with 35% H_2O_2 the reaction was first order in both the catalyst and substrate, the order in the oxidant being changed from first to zero with increasing H_2O_2 concentration. Both ^{31}P NMR and kinetic data are consistent with mechanism, including fast dissociation of **1** to the monomer (**2**), the equilibrium formation of active hydroperoxo complex $PW_{11}TiOOH$ (**B**) from **2**, and interaction of **B** with thioether. The rate-limiting steps are the formation of **B** and the interaction of **B** with sulfide at low and high H_2O concentrations, respectively. The kinetic study of stoichiometric reaction between **B**, generated *in situ* from inactive side-on peroxocomplex $PW_{11}TiO_2$ (**A**), and thioethers showed first order dependence on both **B** and sulfide concentration, thus indicating that no binding of thioether to Ti(IV) occurs. The lack of Hammett type correlation and specific products obtained in oxidation of benzyl phenyl sulfide allowed to rule out electrophilic oxygen transfer and suggest a mechanism that involves the formation of a thioether cation radical intermediate.

NOVEL TITANIUM-CONTAINING DIMER HETEROPOLYTUNGSTATE: SYNTHESIS, CHARACTERIZATION AND CATALYSIS OF H_2O_2-BASED THIOETHER OXIDATION

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Inorg. Chem., 39 (2000) pp. 3828-3837.

The previously unknown titanium(IV)-containing μ-hydroxo dimeric heteropolytungstate $(Bu_4N)_7[\{PTiW_{11}O_{39}\}_2OH]$ (TBA salt of H**1**) has been synthesized, starting from $H_5PTiW_{11}O_{40}$, and characterized by elemental analysis, multinuclear (^{31}P, ^{17}O, ^{183}W) NMR, IR, FAB-MS, cyclic voltammetry and potentiometric titration. ^{31}P NMR reveals that H**1** (δ -12.76) readily forms in MeCN from the Keggin monomer (POM), $PTiW_{11}O_{40}^{5-}$ (**2,** δ -13.34), upon addition of 1.5 equiv of H^+, via the protonated species, $P(TiOH)W_{11}O_{39}^{4-}$ (H**2,** δ -13.44). The ratio of H**1**, **2** and H**2**, which are present in equilibrium in MeCN solution at 25 °C, depends on the concentration of both H^+ and H_2O. The Ti-O-Ti linkage readily reacts with nucleophilic reagents, such as H_2O and ROH to yield monomeric Keggin derivatives. μ-Hydroxo dimer H**1** shows higher catalytic activity than **2** for thioether oxidation by hydrogen peroxide in acetonitrile. The reaction proceeds readily at room temperature and affords the corresponding sulfoxide and sulfone in ca. quantitative yield. The addition of H_2O_2 to H**1** or H**2** results in the formation of a peroxo complex, most likely, the hydroperoxo complex $P(TiOOH)W_{11}O_{39}^{4-}$ (**I**), which has ^{31}P NMR resonance at -12.43 ppm. The rate of the formation of **I** is higher from H**2** than from H**1**. When H**1** is used as a catalyst precursor, the rate of the thioether oxidation as well as the rate of the peroxo complex formation increases with increasing of H_2O concentration, which favors the cleavage of H**1** to H**2**. H_2O_2 in MeCN slowly converts **2** to another peroxotitanium complex, $P(TiO_2)W_{11}O_{39}^{5-}$ (**II**), which has ^{31}P NMR resonance at -12.98 ppm. Peroxo complexes **I** and **II** differ in their protonation state and interconvert fast on the ^{31}P NMR time scale. Addition of 1 equiv of H^+ completely converts **II** to **I**, while 1 equiv of OH^-

completely converts **I** to **II**. ^{31}P NMR confirms that **I** is stable under turnover conditions (thioether, H_2O_2, MeCN). Contrary to two-phase systems like dichloroethane/aqueous H_2O_2, no products resulting from destruction of the Keggin POM were detected in MeCN in the presence of H_2O_2 (a 500-fold molar excess). The reactivity of **I**, generated *in situ* from **II** by adding 1 equiv of H^+, towards organic sulfides under stoichiometric conditions was confirmed using both ^{31}P NMR and UV-vis spectroscopy. This is a rare demonstration of the direct stoichiometric oxidation of an organic substrate by a titanium peroxo complex.

ALKENE AND THIOETHER OXIDATIONS WITH H_2O_2 OVER Ti-CONTAINING MESOPOROUS MESOPHASE CATALYSTS

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J. Molec. Catal. A: Chemical, 158 (2000) pp. 417-421.

Well-organized Ti-containing mesoporous mesophase materials (Ti-MMM) have been synthesized by hydrothermal synthesis using $C_{16}H_{33}N(CH_3)_3Br$ and characterized by elemental analysis, IR, DRS-UV, XRD, and N_2 adsorption. Catalytic properties of these materials in alkene and thioether oxidations with aqueous H_2O_2 in MeCN have been studied and compared with those of Ti-HMS. The Ti-MMM catalysts with the Si/Ti atomic ratio varied in the range of 49÷124 showed the highest catalytic activities in alkene oxidation. Both structure of a silicate matrix and a degree of isolation of titanium ions in it are crucial factors determining catalytic activity of Ti-MMM. For thioether oxidation the structural perfection of Ti-MMM catalysts is less important. No leaching of titanium ions occurs during both reactions. The oxidation process proved to be true heterogeneous.

COUPLING OF PHENOL WITH KETONES IN THE PRESENCE OF HETEROPOLY ACIDS WITH DIFFERENT STRUCTURES AND COMPOSITIONS

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Kinetics & Catalysis, 41 (2000) pp. 767-770.

The reactions of phenol coupling with ketones MeCOR (R=CH_3, C_2H_5, C_3H_7, and C_4H_9) are studied in the presence of heteropoly acids with different structures and compositions in toluene solutions ([PhOH]/[MeCOR]=(28)/1 mol/mol; 50-70°C) with thioglycolic acid added as a promoter. The reaction rate depends on ketone and heteropoly acid, and the yield of bisphenols is as high as 24–72%. The reaction orders are 0.68, 0.77, and 0.97 with respect to $H_6P_2W_{21}O_{71}$, $H_3PW_{12}O_{40}$, and $H_4SiW_{12}O_{40}$, respectively, and the activation energies are 25.1, 21.0, and 20.6 kcal/mol, respectively. Heteropoly acids of the Dawson structure exhibited the highest activity.

ALKALINE HYDROLYSIS OF KEGGIN HETEROPOLY ACIDS IN THE PRESENCE OF METAL CARBONATES

G.M. Maksimov

Russ. J. Inorg. Chem., 45 (2000) pp. 1451-1452.

The reactions of the heteropoly acids (HPAs) $H_3PM_{12}O_{40}$ and $H_4SiM_{12}O_{40}$ (M=Mo, W) in aqueous solutions with Ni(II), Mg(II), Co(II), Cu(II), Zn(II), Mn(II), Ca(II), Cd(II), La(III), and Ce(III) carbonates were studied by IR and ^{31}P NMR spectroscopy. The major reaction products are the complexes $[(PM_{11}O_{39})_2Me]^{11-}$ and $[(SiM_{11}O_{39})_2Me]^{12-}$ for La and Ce carbonates (Me is the metal ion from the carbonate) and $[PM_{11}MeO_{39}]^{5-}$ and $[SiM_{11}MeO_{39}]^{6-}$ for the other carbonates; the Me ions also function as the salt-forming cations.

ACTIVE METAL SPECIES ASSEMBLED WITH HETEROPOLY TUNGSTATE ANION $PW_9O_{34}^{9-}$ FOR LIQUID PHASE HYDROCARBON OXIDATION

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J. Molec. Catal. A: Chemical, 158 (2000) pp. 429-433.

Monometallic $[Pd_3(PW_9O_{34})_2]^{12-}$, $[Pd_3(PW_9O_{34})_2Pd_nO_xH_y]^{q-}$ (where on the average n=3), bimetallic $[Pd_2Cu(PW_9O_{34})_2]^{12-}$, $[Pd_2Fe(PW_9O_{34})_2]^{11-}$, $[PdFe_2(PW_9O_{34})_2]^{10-}$ and a mixture of $[Pd_3(PW_9O_{34})_2Pd_nO_xH_y]^{q-}$ ($n_{av}\approx 10$) + $[(VO_3)(PW_9O_{34})_2]^{9-}$ complexes were prepared and characterized by NMR ^{31}P, ^{183}W, ^{51}V and IR spectroscopy. The complexes were tested in catalysis of O_2+H_2 reaction and benzene oxidation to phenol with O_2/H_2. Effectiveness of the catalytic performance depended on the composition of the complexes. Bimetallic Pd(II)-Fe(III) complexes were several times more active in phenol production than Pd(II) monometallic system.

Studies on Selective Catalytic Oxidation

HETEROGENEOUS SELECTIVE OXIDATION OF FORMALDEHYDE ON OXIDE CATALYSTS: *IN SITU* FTIR STUDY OF FORMALDEHYDE SURFACE SPECIES ON A VTiO CATALYST AND OXYGEN EFFECT

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T.V. Andrushkevich, E.S. Stoyanov

Kinetics & Catalysis, 41 (2000) pp. 546-552.

The interaction of formaldehyde with a highly selective V–Ti–O catalyst for the oxidation of formaldehyde to formic acid is studied by Fourier-transform infrared (FTIR) spectroscopy at 70–200°C. In a flow of formaldehyde/oxygen mixture and in a mixture without oxygen at optimal temperatures for formic acid formation (100–140°C), methoxy groups and other oxygenates are formed in small amounts. These are two bidentate formates and covalently bound monodentate formate. The fact that similar oxygenates are observed independently of the presence of oxygen in the reaction mixture suggests the participation of the catalyst oxygen in their formation. Oxygen accelerates the desorption of bidentate formates. Bidentate formates of one type decompose in a flow of air at 100–150°C, and bidentate formates of the other type decompose at 170–200°C.

SURFACE INTERMEDIATES IN SELECTIVE FORMALDEHIDE OXIDATION ON V-Ti-O CATALYST IDENTIFIED WITH *IN SITU* FTIR SPECTROSCOPY

G.Ya. Popova, Yu.A. Chesalov, T.V. Andrushkevich,
I.I. Zakharov, E.S. Stoyanov

J. Molec. Catal. A: Chemical, 158 (2000) pp. 345-348.

Formaldehyde oxidation to formic acid on V-Ti-O catalyst was studied in a flow-circuit setup with a differential reactor and in the IR cell. Surface intermediates leading to formic acid formation were identified. Catalyst calcination temperature was varied to study its effect on catalyst performance and surface species structure.

FORMATION OF ACTIVE STATE IN VANADIUM-TITANIUM OXIDE SYSTEM REGARDING TO REACTION OF OXIDATION OF β-PICOLINE TO NICOTINIC ACID

E.M. Al'kaeva, T.V. Andrushkevich,
G.A. Zenkovets, G.N. Kryukova, S.V. Tsybulya

Catal. Today, 61 (2000) pp. 249-254.

Binary vanadia-titania catalysts comprising 5-75 wt.% of V_2O_5 and 95-25 wt.% of TiO_2, pretreated at the temperature ranging between 300 and 700°C, were studied as heterogeneous catalysts for oxidation of β-picoline at 250°C, and inlet concentrations of the following components (vol.%): 1% of 3-picoline, 20% of oxygen, 30% of steam. Nicotinic acid, 3-pyridinecarbaldehyde and CO_2 were the reaction products. The most active state for oxidation of 3-picoline into nicotinic acid was shown to result from formation of coherent interface between V_2O_5 and TiO_2 (anatase) crystallites. This state was generated at the temperature particular for each composition and persist below the temperature of the anatase to rutile transition.

OXIDATIVE AMMONOLYSIS OF METHYLPYRAZINE OVER BINARY CATALYTIC SYSTEMS:
3. PHOSPHORUS MOLYBDENUM SYSTEM: CATALYTIC PROPERTIES AND THE ACTIVE COMPONENT

V.M. Bondareva, T.V. Andrushkevich,
N.N. Chumachenko, R.I. Maksimovskaya,
L.M. Plyasova, V.V. Malakhov, L.S. Dovlitova,
E.B. Burgina, G.S. Litvak

Kinetics & Catalysis, 41 (2000) pp. 222-230.

The phase composition of the binary phosphorus–molybdenum system with a Mo/P ratio of 3–24.5 and its catalytic properties in the reaction of oxidative ammonolysis of methylpyrazine are studied. X-ray amorphous phases of molybdenyl phosphate and phosphorus modified molybdenum trioxide are active in the formation of pyrazinonitrile.

AMMOXIDATION OF METHYLPYRAZINE OVER BINARY OXIDE SYSTEMS:
IV. A VANADIA-TITANIA SYSTEM

V.M. Bondareva, T.V. Andrushkevich, O.B. Lapina,
V.V. Malakhov, L.S. Dovlitova, A.A. Vlasov

Kinetics & Catalysis, 41 (2000) pp. 670-678.

The catalytic properties of vanadia–titania catalysts in methylpyrazine ammoxidation are studied.

The activity monotonically increases on changing the concentration from pure titania to pure vanadia, and the yield of methylpyrazine passes through a broad maximum corresponding to a V_2O_5 concentration from 10 to 75 wt %. The active sites of binary catalysts contain V^{5+} cations in a substantially distorted octahedral environment of oxygen atoms, which are strongly bound to anatase, likely due to the formation of V–O–Ti bonds.

AMMOXIDATION OF METHYLPYRAZINE OVER V-Ti OXIDE SYSTEM

V.M. Bondareva, T.V. Andrushkevich, O.B. Lapina

Catal. Today, 61 (2000) pp. 173-178.

The catalytic properties of vanadium-titanium oxide system in ammoxidation of methylpyrazine have been studied. Catalytic activity increases monotonically and yield of selective products passes a wide maximum in the range of V_2O_5 content form 10 to 75 wt.% with increase in the V/Ti relation. The active centers of binary catalysts include V^{5+} cations with distorted octahedral coordination strongly bounded with titania apparently owing to formation of V-O-Ti bonds.

EFFECT OF POTASSIUM DOPING ON THE STRUCTURAL AND CATALYTIC PROPERTIES OF V/Ti-OXIDE IN SELECTIVE TOLUENE OXIDATION

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V.I. Zaikovskii, O.B. Lapina, A.A. Ivanov,
S.I. Reshetnikov, A. Renken* (*Institute of Chemical Engineering, Swiss Federal Institute of Technology, Lausanne, Switzerland)

Appl. Catal. A: General, 20 (2000) pp. 243-250.

Small addition of potassium to V/Ti-oxide catalyst (K:V=0.19), consisting of 3.7 monolayer VO_x, increased activity and selectivity in partial oxidation of toluene. In order to elucidate the nature of vanadia species formed on the surface of V/Ti-oxide upon potassium doping, the catalysts were studied by transient kinetics method. The transient product responses during toluene oxidation by the oxygen present in the catalyst were compared for K-doped and non-doped samples. The formation of CO_2 decreased and formation of benzaldehyde increased with addition of potassium. This suggests a lower surface concentration of electrophilic oxygen (O^-, O^-_2), which is usually responsible for the deep oxidation, and a higher concentration of nucleophilic oxygen (O^{2-}), responsible for the partial oxidation.

These catalysts were characterized by means of HRTEM, FT-Raman spectroscopy and ^{51}V NMR. Potassium addition introduces a disorder in the crystalline structure of bulk V_2O_5 with TiO_2 was facilitated upon K-doping, leading to the increased formation of monomeric vanadia species, which are the active sites in toluene partial oxidation to benzaldehyde.

FORMATION OF ACTIVE SITES FOR SELECTIVE TOLUENE OXIDATION DURING CATALYST SYNTHESIS VIA SOLID-STATE REACTION OF V_2O_5 WITH TiO_2

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J. Catal., 193 (2000) pp. 145-153.

Interaction of V_2O_5 with TiO_2 during the preparation of V/Ti oxide catalysts via solid-state reaction has been studied by means of *in situ* FT-Raman spectroscopy, HRTEM and XPS. This interaction results in the formation of monomeric vanadia species with vanadium in tetrahedral coordination. The bridging oxygen in the V-O-Ti bond is suggested to be responsible for the catalytic activity during the partial oxidation of toluene. The formation of the monomeric vanadia species correlates with the improved catalyst performance, characterized by reaction rate and selectivity to benzaldehyde and benzoic acid. Mechanical activation by intensive grinding of V_2O_5/TiO_2 mixture via ball milling was necessary for the interaction of the oxides during the calcination. The monomeric species formation was observed at a temperature as low as 523 K. The dynamics of V_2O_5/TiO_2 interaction strongly depends on the presence of moisture during the calcination. In dry oxidative atmosphere, a part of the monomeric species is rapidly formed. During the calcination in humid oxidative atmosphere, quick amorphization of bulk crystalline V_2O_5 was observed followed by slow formation of the monomeric vanadia species.

THE RADICALS GENERATION IN THE METHANOL OXIDATION ON A Pt-CONTAINING CATALYSTS. INFLUENCE OF SUPPORT ACIDIC PROPERTIES

I.V. Malakhova, V.K. Ermolaev, E.A. Paukshtis

J. Molec. Catal. A: Chemical, 158 (2000)
pp. 439-442.

Gas phase radicals, formed during methanol oxidation, have been investigated for series of Pt-containing catalysts with different support acidic properties, using matrix isolation method. Generation rates and activation energies were determined. It was estimated that strength and concentration of active surface sites play an important role in radicals generation.

EFFECT OF PORTIONWISE ADDITION OF OXIDANT IN ASYMMETRIC VANADIUM-CATALYSED SULFIDE OXIDATION

N.N. Karpyshev, O.D. Yakovleva, E.P. Talsi, K.P. Bryliakov, O.V. Tolstikova, A.G. Tolstikov

J. Molec. Catal. A: Chemical, 157 (2000) pp. 91-95.

Portionwise addition of hydrogen peroxide markedly augments enantioselectivity of sulfide to sulfoxide oxidation catalyzed by vanadium (IV) - Shiff base complexes, and this effect cannot be explained by temperature fluctuations. ^{51}V NMR spectra of reaction mixture detect two chiral peroxo complexes and one achiral diperoxo compound.

HYDROXIDES OF TRANSITION METALS AS ARTIFICIAL CATALYSTS FOR WATER OXIDATION TO DIOXYGEN

G.L. Elizarova, G.M. Zhidomirov, V.N. Parmon

Catal. Today, 58 (2000) pp. 71-88.

Hydroxides of transition metals cations like Fe(III), Co(III), Mn(III), Ru(IV) appear to be efficient artificial catalysts in oxidation of water to O_2. The paper describes some catalytic properties of these hydroxides. The hydroxide-based catalysts for the water oxidation can be obtained in three modification: bulky (individual and binary), supported on the ion exchange resins or conventional oxide supports (SiO_2, TiO_2, Al_2O_3, zeolites), and colloidal catalysts stabilized by starch. The possible mechanism of the catalytic reaction including the stage of the formation of peroxocomplexes as intermediates is under discussion. Some similarities are drawn between the catalytic properties of hydroxide catalysts and those of manganese-based oxygen evolving complex of the Photosystem II of green plants.

Studies on Selective Catalytic Reduction

NANOCOMPOSITES BASED UPON ALUMINA AND ZIRCONIA PILLARED CLAYS LOADED WITH TRANSITION METAL CATIONS AND CLUSTERS OF PRECIOUS METALS: SYNTHESIS, PROPERTIES AND CATALYSIS OF NO_X SELECTIVE REDUCTION BY HYDROCARBONS

V.A. Sadykov, R.V. Bunina, G.M. Alikina, V.P. Doronin, T.P. Sorokina, D.I. Kochubey, B.N. Novgorodov, E.A. Paukshtis, V.B. Fenelonov, A.Yu. Derevyankin, A.S. Ivanova, V.I. Zaikovskii, T.G. Kuznetsova, S.A. Beloshapkin, V.N. Kolomiichuk, L.M. Plyasova, V.A. Matyshak*, A. Konin*, A.Ya. Rozovskii, V.F. Tretyakov**, T.N. Burdeynaya**, M.N. Davydova**, J.R.H. Ross***, J.P. Breen***, F.C. Meunier***** (*Semenov Institute of Chemical Physics, Moscow, Russia; **Topchiev Institute of Petrochemical Synthesis, Moscow, Russia; ***University of Limerick, Limerick, Ireland)

Mat. Res. Soc. Symp. Proc., 581 (2000) pp. 435-440.

Thermally stable alumina and zirconia pillared clays loaded with copper and cobalt cations and silver nanoparticles were synthesized. The structural and surface features of these nanosystems were studied and compared with those of bulk analogs - partially stabilized zirconias and γ-alumina loaded with the same active components. Specificity of the catalytic properties of nanocomposites in the reactions of nitrogen oxides reduction by propane, propylene and decane in the excess of oxygen appears to be determined both by the degree of interaction between pillars and active components and the type of reducing agent.

Cu, Co, Ag -CONTAINING PILLARED CLAYS AS CATALYSTS FOR THE SELECTIVE REDUCTION OF NO_X BY HYDROCARBONS IN AN EXCESS OF OXYGEN

G.A. Konin*, A.N. Il'ichev*, V.A. Matyshak*, T.I. Khomenko*, V.N. Korchak*, V.A. Sadykov, V.P. Doronin, R.V. Bunina, G.M. Alikina, T.G. Kuznetsova, E.A. Paukshtis, V.B. Fenelonov, V.I. Zaikovskii, A.S. Ivanova, S.A. Beloshapkin, A.Ya. Rozovskii, V.F. Tretyakov**, J.R.H. Ross**, J.P. Breen***** (*Semenov Institute of Chemical Physics, Moscow, Russia; **Topchiev Institute of Petrochemical Synthesis, Moscow, Russia; ***University of Limerick, Limerick, Ireland)

Proceedings of the "CAPOC-5", V. 2 (2000) pp. 97-106.

Zirconia and alumina pillared montmorillonite clays containing transition metal cations and Ag appear to be promising as HC-SCR catalysts due to their

- high thermal stability;
- high catalytic activity;
- high selectivity in the reduction of NO_x by hydrocarbons in an excess (up to 20%) of oxygen.

Structural features and surface properties of zirconia and alumina pillars located between the clay layers and loaded with transition metal cations and silver were shown to differ appreciably from those of the bulk analogs due to a stronger oxide-oxide and/or oxide-metal interaction. It is reflected in the catalytic performance of these systems in the NO_x selective reduction by hydrocarbons helping to obtain some active systems interesting for the practical application.

INVESTIGATION OF THE STATE OF COPPER IN SUPPORTED COPPER-TITANIUM OXIDE CATALYSTS

O.V. Komova, A.V. Simakov, V.A. Rogov, T.A. Nikoro, D.I. Kochubey, G.V. Odegova, V.V. Kriventsov, E.A. Paukshtis, V.A. Ushakov, N.N. Sazonova

J. Molec. Catal. A: Chemical, 161 (2000) pp. 191-204.

Supported copper-titanium oxide catalysts have been studied by IR spectroscopy, XRD, UV-visible diffuse reflectance spectroscopy, ESR, TPR with hydrogen and EXAFS. Different states of Cu^{2+} ions have been found on the surface of TiO_2. The ratio between these states depends on the copper concentration and catalyst preparation method. Chain structures are formed due to the interaction of Cu^{2+} ions with TiO_2. Their concentration and geometry of their nearest oxygen environment are determined by the structure of anatase faces. Some of these surface-stabilized Cu^{2+} ions are nucleation centers of oxide clusters. A noticeable growth of bulk CuO phase is observed after the completion of the formation of chain structures and oxide clusters. A quantitative estimation of the concentration of these copper forms in the catalysts is reported. For supported copper-titanium oxide catalysts, chain forms of Cu^{2+} ions are shown to be the most active forms of copper in NO SCR with ammonia and CH_4 oxidation.

RATE-DETERMINING STAGE IN NO SCR WITH PROPANE ON LOW-EXCHANGED Cu-ZSM-5 CATALYST

E.V. Rebrov, A.V. Simakov, N.N. Sazonova, E.S. Stoyanov

Catal. Lett., 64 (2000) pp. 129-134.

The kinetics of the NO SCR with propane has been studied on a low-exchanged Cu-ZSM-5 catalyst. The kinetic analysis of the reaction has revealed that there are two temperature regions with significantly different reaction pathways. Below 300°C the reaction is determined mostly by NO content in the gas phase as the propane plays an important role at more high temperatures. The study of the kinetics of individual reaction stages (2-nitrosopropane isomerization to acetone oxime and reaction of adsorbed acetone oxime with gaseous NO) has shown that the NO reaction with acetone oxime is the rate-determining stage in the whole chain of transformations leading to the formation of molecular nitrogen in the low-temperature region.

Studies on Electrocatalytic Processes

EFFECT OF NON-FARADAIC ELECTROCHEMICAL MODIFICATION OF CATALYTIC ACTIVITY

V.D. Belyaev, T.I. Politova, V.A. Sobyanin

Solid State Ionics, 135 (2000) pp. 721-726.

The present paper briefly reviews researches on non-Faradaic electrochemical modification of catalytic activity (NEMCA effect) and discusses CO oxidation in a solid oxide electrolyte cell under the NEMCA conditions basing on the chain reaction mechanism involving electrochemically generated oxygen species.

GAS-PHASE ELECTROCATALYSIS: METHANE OXIDATION TO SYNGAS IN A SOLID OXIDE FUEL CELL REACTOR

V.A. Sobyanin, V.D. Belyaev

Solid State Ionics, 135 (2000) 747-752.

Electrocatalytic methane-to-syngas oxidation over metal-based electrodes in SOFC reactor is discussed. The main attention is focused on the behavior of Pt and Ni electrodes, which demonstrate high electrocatalytic activity towards formation of syngas from methane.

IN SITU EXAFS STUDY OF Ru-CONTAINING ELECTROCATALYSTS OF OXYGEN REDUCTION

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Nuclear Instrum. & Methods in Phys. Research A, 48 (2000) pp. 323-326.

The series of Ru chalcogenide compounds is obtained by varying the nature of the chalcogen with the transition metal (Ru) matrix. The EXAFS technique reveals that the electrocatalytic center is Ru in a cluster matrix. Furthermore, a reversible change in the structure of the active center as a function of the applied electrode potential appears.

ELECTROCATALYTIC OXIDATION OF ETHYLENE GLYCOL ON DISPERSED Pt: DETERMINATION OF THE REACTION PRODUCTS

O.V. Cherstyuk, E.R. Savinova, L.A. Kozhanova*, G.N. Kryukova, V.N. Parmon (*Limnological Institute, Irkutsk, Russia)

React. Kinet. & Catal. Lett., 69 (2000) pp. 331-338.

Comparative studies of electrocatalytic ethylene glycol oxidation on bulk and dispersed Pt in acidic aqueous solutions have been performed. A quantitative method has been developed to determine all organic oxidation products using high-performance liquid chromatography with appropriate derivatising reagents.

ON THE MECHANISM OF Ag(111) SUB-MONOLAYER OXIDATION: A COMBINED ELECTROCHEMICAL, *IN-SITU* SERS AND *EX-SITU* XPS STUDY

E.R. Savinova, D.Yu. Zemlyanov*, B. Pettinger, A. Scheybal**, R. Schloegl**, K. Doblhofer**** (*Worcester Polytechnic Institute, Department of Chemical Engineering, Worcester, USA; **Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany)

Electrochim. Acta, 46 (2000) pp. 175-183.

In the present work *in-situ* surface enhanced Raman spectroscopy (SERS), *ex-situ* X-ray photoelectron spectroscopy (XPS) and ultraviolet photoelectron spectroscopy (UPS) are used to study the interface between a Ag(111) electrode and an alkaline electrolyte. Formation of a number of potential-dependent adsorbates is observed above the point of zero charge (E_{pzc}) of the Ag electrode. These are: surface OH groups ($OH^{\gamma-}_{ads}$), surface oxide-like species ($O^{\delta-}_{ads}$) and OH groups, incorporated in the bulk of the electrode (OH_{bulk}). Electrochemisorbed hydroxide species show by the appearance of Raman bands at 540 – 560 cm^{-1} and at 803 – 819 cm^{-1}, attributed to Ag-OH stretching and AgO-H bending vibrations respectively. Strong isotope shift of the Raman bands towards lower frequencies is observed in D_2O solutions, proving their assignment. The $O^{\delta-}_{ads}$, $OH^{\gamma-}_{ads}$ and OH_{bulk} species are characterised by the O 1s peaks at ca. 529.5, 531.6 and 532.8 eV, respectively. Formation of the above-mentioned species is verified also by the UP spectra of the emersed electrodes, showing the bands at 3.0 eV typical for the oxide-like adsorbates and 9.0 and 11.1 eV for hydroxo-groups. The $OH^{\gamma-}_{ads}$ and $O^{\delta-}_{ads}$ species are negatively charged, as evidenced by the adsorption of Na^+ on the Ag electrode positive to the E_{pzc}. A mechanism of the Ag(111) premonolayer oxidation is suggested on the basis of combined evidence from cyclic voltammetry, *in-situ* SERS, *ex-situ* XPS and UPS

ELECTROCATALYTIC PROPERTIES OF PLATINUM ANCHORED TO THE SURFACE OF HIGHLY ORIENTED PYROLYTIC GRAPHITE

E.R. Savinova, N.P. Lebedeva, P.A. Simonov, G.N. Kryukova

Russ. J. Electrochem., 36 (2000) pp. 952-959.

Nano-sized particles of platinum deposited on highly oriented pyrolytic graphite (HOPG) electrolessly (average size d = 3.4 nm) or electrochemically (d = 20 nm) and polycrystalline platinum are compared. The dispersed electrodes exhibit special features in the oxidation of ethylene glycol and adsorbed carbon monoxide. In particular, they reduce the overpotential of these processes. Possible reasons for the observed distinctions are discussed. The potential cycling leads to coalescence of nano-sized Pt particles on HOPG. As a result, their size distribution expands, and the distribution maximum shifts towards large sizes (d = 6.4 nm). This seriously complicates use of Pt/HOPG as a model electrode for investigating the size effect.

EFFECT OF SILICA POROUS STRUCTURE ON PROPERTIES OF COMPOSITE ELECTROLYTES BASED ON $MeNO_3$ (Me=Rb, Cs)

V.G. Ponomareva*, G.L. Lavrova*, L.G. Simonova (*Institute of Solid State Chemistry and Mechanochemistry, Novosibirsk, Russia)

Solid State Ionics, 136-137 (2000) pp. 1279-1283.

Properties of $RbNO_3$ and $CsNO_3$ in (1-x)$MeNO_3$-xSiO_2 (x=0-0.9) nanocomposite solid electrolytes were studied by X-ray powder diffraction, differential scanning calorimetry methods and conductivity measurements. The used highly-dispersed silicas with narrow pore size distribution were different in their specific surface areas (13-580 m^2/g) and pore size (R=14-1000 Å). The composite conductivity was shown to exceed that of individual salts more than 1.5-4 orders of magnitude and to be maximum at x=0.5-0.7. In nanocomposites based on alkali nitrates and silica the "dimensional effect" was observed. The properties of composites depended markedly on pore size of silica. The optimum pore size of heterogeneous dopant was in a range of 35-100 Å, where the most composite conductivity increase took place and thermodynamic and structural properties of ionic salts changed markedly. For composites based on these silicas the enthalpies of $RbNO_3$ ($CsNO_3$) phase transitions and melting decreased considerably. The ionic component became either partially or completely amorphous (in particular with x increase). The $MeNO_3$ state changed slightly when the SiO_2 pore size was 1000 Å. In systems with pore size 14 Å both crystalline low temperature $RbNO_3$ (IV) and amorphous salt were observed.

THE CHEMICAL AND ADSORPTION EFFECTS OF FOREIGN MOLECULES ON THE PROPERTIES OF HIGH-TEMPERATURE SUPERCONDUCTORS

L.L. Makarshin, D.V. Andreev, V.N. Parmon

Russ. Chem. Rev., 69 (2000) pp. 279-305.

Data on the effect of adsorption and intercalation of foreign molecules on the properties of high-temperature superconducting materials and on the reciprocal effect of superconductivity on the electronic state of adsorbed molecules are considered. Particular attention is given to the analysis of experimental conditions and interpretation of the results obtained. An effect of adsorbed molecules on the electrophysical state and the critical parameters of superconductors is noted. Specific features of the interaction between the phases in the superconducting state and the external molecules are discussed. The bibliography includes 280 references.

EFFECT OF THE DPPH RADICAL ADSORPTION ON SUPERCONDUCTING PROPERTIES OF BISMUTH HTSC CERAMICS

L.L. Makarshin, V.N. Parmon

Chem. Phys. Lett., 327 (2000) pp. 176-180.

Measuring the AC susceptibility and registering the ESR spectra of the stable 1,1-diphenyl-2 picryl-hydrosyl (DPPH) radical at 77.4-125 K the effect of the radical on the current properties of the intergranular contacts in the superconducting ceramics $Bi_{1.8}Pb_{0.3}Sr_{1.9}Ca_{2.8}Cu_{3.4}O_y$ has been studied. Critical current in the ceramics is decreased by the magnetic field generated by the radical spin. The effect of the field on the critical current corresponds to the location of the adsorbed radical at a distance of 56 Å from the superconducting phase.

New Results in Studying Photocatalytic and Related Processes

PHOTOINDUCED PHENOMENA ON THE SURFACE OF WIDE-BAND GAP OXIDE

A.M. Volodin

Catal. Today, 58 (2000) pp. 103-114.

This article reviews papers devoted to the investigation of photoinduced processes on non-semiconductor oxide catalysts. The main results of ESR *in situ* studies of such systems are presented. Wide-band-gap oxides are shown to constitute a new and very promising class of photocatalysts capable of functioning under illumination with visual light. It is shown that in many cases the light is initially absorbed by charge-transfer complexes with the following generation of ion-radical intermediates with high reactivity.

A very important feature of photoinduced reactions in the absorption band of charge-transfer complexes is a significant shift of their red edge to longer wavelengths in comparison with similar processes in homogeneous systems. In many cases, the formation of such complexes is caused by the existence of strong acceptor or donor sites typical for many oxide catalysts with pronounced acidic or basic properties.

DESTRUCTIVE PHOTOADSORPTION OF FREONS ON ATMOSPHERIC AEROSOLS

V.N. Parmon, V.S. Zakharenko

Zeitschrift fur Physikalische Chemie, 213 (1999) pp. 9-16.

Under discussion is possible impact of the solar light driven processes on the natural nontechnogeneous remediation of the Earth's atmosphere from freons. The paper concerns an expected role of photocatalytic and photosorption processes on tropospheric aerosols in Global Chemistry of the Earth's atmosphere as well as recent experimental data on photoadsorption phenomena over alkaline earth metal oxides like MgO and CaO at conditions of *real* Earth's atmosphere. Interaction of some freons like CF_3CH_2F (freon 134a) and CHF_2Cl

(freon 22) with the ambient air-exposed surface of magnesium oxide and calcium hydroxycarbonate under mild UV radiation, which corresponds to solar light in the troposphere, is shown to result in their efficient irreversible destructive adsorption. The above photoactivity appears to be related with an optical absorption, detected at wavelengths ranging within 300-400 nm and caused presumably by some surface compounds. The photoadsorption is observed for H-containing freons only while for hydrogen-free ozone-depleting freons like CF_2Cl_2 (freon 12) and $C_2F_3Cl_3$ (freon 113) it is not detected. At the photostimulated adsorption, fluorine and chlorine atoms seem to substitute oxygen atoms in the magnesium oxide lattice and hydroxyl groups of calcium hydroxycarbonates. It was found that the observed photoadsorption phenomena might be related also with the presence of a certain amount of N_2O natively adsorbed on the alkaline earth metal oxides exposed to ambient air.

PHOTOADSORPTION AND PHOTOCATALYTIC PROCESSES AFFECTING THE COMPOSITION OF THE EARTHS ATMOSPHERE: II. DARK AND PHOTOSTIMULATED ADSORPTION OF FREON 22 (CHF_2Cl) ON MgO

V.S. Zakharenko, V.N. Parmon

Kinetics & Catalysis, 41 (2000) pp. 756-759.

The interaction of hydrogen-containing Freon 22 (CHF_2Cl) with the surface of MgO that was held in air both before and after heating at 620 K in the dark or under exposure to soft UV radiation, which corresponded to the solar spectrum in the troposphere, is examined. Up to 1% of a Freon 22 monolayer is adsorbed on the surface of MgO in the dark, and more than 10% of a monolayer was adsorbed under UV irradiation. The photoadsorption activity is not associated with the presence of nitrogen-containing compounds formed by the adsorption of nitrogen oxides from air on the surface of MgO. Magnesium oxide does not adsorb hydrogen-free Freon 12 (CF_2Cl_2) either in the dark or under exposure to UV radiation.

THE COMPARATIVE STUDIES OF TITANIUM DIOXIDE IN GAS-PHASE ETHANOL PHOTOCATALYTIC OXIDATION BY THE FTIR *IN SITU* METHOD

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(*Novosibirsk State University, Novosibirsk, Russia)

Appl. Catal. B: Environmental, 24 (2000) L7-L12.

Gas-phase ethanol photocatalytic oxidation on the series of TiO_2 samples has been studied by the FTIR *in situ* method. The TiO_2 samples were prepared by the usual method and they possessed similar physicochemical properties (porosity, specific area), but were found to have different photocatalytic activities. The acidity and concentration of the Lewis centers have been measured. The TiO_2 photocatalytic activity has been found to correlate with the surface acidity, and the Ti^{3+} and carbonate surface concentrations.

KINETICS OF THE PHOTOCATALYTIC OXIDATION OF GASEOUS ACETONE OVER PLATINIZED TITANIUM DIOXIDE

A.V. Vorontsov, I.V. Stoyanova, D.V. Kozlov*, V.I. Simagina, E.N. Savinov (*Novosibirsk State University, Novosibirsk, Russia)

J. Catal., 189 (2000) pp. 360-369.

The photocatalytic oxidation of acetone is investigated in a flow-circulating reactor over Pt/TiO_2 prepared by photodeposition (Pt/TiO_2-P) as well as by reduction with $NaBH_4$ (Pt/TiO_2-C). Compared to untreated TiO_2, Pt/TiO_2-P is less active and Pt/TiO_2-C more active at 40-120°C, water concentration of 4500 ppm, and light intensity of 1.10×10^{-6} E/(min cm^2). The increased activity of Pt/TiO_2-C is related to the stronger adsorption of acetone and higher rate constant, as revealed by dependence of the reaction rate on concentration. Adsorption constants obtained from adsorption isotherms are significantly lower than those constants obtained from the dependence of the rate on acetone concentration. This suggests the presence of acetone photoadsorption during photocatalytic oxidation. Platinized samples did not demonstrate steady state deactivation, which was observed over TiO_2 at temperatures above 100°C. However, there was a decrease in the oxidation rate while reaching steady state after an increase of temperature to 80°C and above. Apparent activation energy of photocatalytic oxidation over platinized samples was 10-13 kJ/mol; the apparent activation energy of thermal acetone oxidation was 84 kJ/mol for Pt/TiO_2-P and about 40 kJ/mol for Pt/TiO_2-C. At 80-140°C, photoinduced oxidation could occur on Pt particles, as shown by acetone photoinduced oxidation over $Pt/\gamma\text{-}Al_2O_3$. The lack of deactivation of Pt/TiO_2 above 100°C may be related to the modification of the TiO_2 surface during Pt deposition because TiO_2 treated with $NaBH_4$ demonstrated a higher deactivation temperature. The dependence of activity on Pt content in Pt/TiO_2-C had a peak at Pt content of about 0.1 wt%. The TiO_2 used in this study had higher adsorption and rate constants compared to TiO_2 Degussa P25. An estimate showed that there were no concentration gradients inside the photocatalyst film under experimental conditions of this study.

VIBROFLUIDIZED- AND FIXED-BED PHOTOCATALYTIC REACTORS: CASE OF GASEOUS ACETONE PHOTOOXIDATION

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Chem. Engin. Sci., 55 (2000) pp. 5089-5098.

Vibrofluidized- and multiple fixed-bed photoreactors were compared under identical operating conditions. The comparison was based on the quantum efficiency for the gas-phase photocatalytic oxidation of acetone using TiO_2 (Hombikat UV 100). Multiple fixed-bed reactor configurations were used, along with a vibrofluidized-bed configuration. Quantum efficiency decreased in the following order: vibrofluidized bed (8.7%) > fixed-bed granules (6.9%) > fixed film bed (5.9%) ~ fixed powdered bed (5.8%). The increased activity of the vibrofluidized-bed could not be attributed to enhanced external mass transport, as all reactor systems used in the present study demonstrated negligible external mass transfer resistances. Instead, the increased activity is most likely credited to the effect of periodic illumination phenomenon taking place because of the random motion of catalyst granules in the fluidized-bed and higher light adsorption of scattered light. The enhanced activity observed for the granular fixed bed could be related to mechanical activation of TiO_2 during the preparation of granules, as well as to increased light adsorption. A maximum of acetone oxidation rate with respect to humidity level was observed. Even at high humidity levels, ultrasound did not affect the rate of gas-phase acetone oxidation. A model has been developed to quantify the absorption of light in a fluidized-bed photoreactor. The model takes into account absorption and single-light scattering and accurately describes the dependence of acetone oxidation rate on the quantity of TiO_2 granules in the vibrofluidized bed.

STUDIES ON THE KINETICS OF INTERFACIAL ELECTRON TRANSFER SENSITIZED BY COLLOIDAL CdS

D.V. Bavykin, E.N. Savinov, V.N. Parmon

J. Photochem. Photobiol. A: Chem., 130 (2000) pp. 57-61.

Flash photolysis was used to study photobleaching of colloidal CdS particles with the controlled size. The rate constant of the photobleaching relaxation was found to depend on the size of the colloidal particles, an increase of the particle size resulting in a decrease of the rate constant. The influence of various electron acceptors on the photobleaching relaxation kinetics was investigated too. The addition of well adsorbing acceptor molecules decreases the initial amplitude of photobleaching and practically does not change the rate constant of the photobleaching relaxation. The photobleaching decay kinetics remains unchanged compared to the photobleaching relaxation kinetics of pure CdS. The addition of acceptor molecules with the small adsorption constant results in an increase of photobleaching relaxation rate constant, while the initial amplitude of photobleaching remains unchanged. Moreover, in the last case the photobleaching decay kinetics became exponential.

PHOTOCATALYTIC STEADY-STATE METHYLVIOLOGEN OXIDATION IN AIR-SATURATED TiO_2 AQUEOUS SUSPENSION: INITIAL PHOTONIC EFFICIENCY AND INITIAL OXIDATION RATE AS A FUNCTION OF METHYLVIOLOGEN CONCENTRATION AND LIGHT INTENSITY

I.N. Martyanov, E.N. Savinov

J. Photochem. Photobiol. A: Chem., 134 (2000) pp. 219-226.

Photocatalytic methylviologen oxidation in TiO_2 aqueous suspension has been studied. The initial photonic efficiency has been found to increase dramatically as the light intensity decreases, approaching 34% at extremely low light intensity. The maximum photonic efficiency does not depend on methylviologen concentration and pH of the solution. Increasing the surface methylviologen concentration by increasing the methylviologen concentration in the solution or varying pH causes the photonic efficiency comes to its maximum value at a higher intensity of incident light. The light intensity affects the shape of the dependencies of initial rate versus methylviologen concentration. The model explaining the experimental data has been examined. Two parameters of this model appear to be able to characterize the material of TiO_2 photocatalysts in a quite wide range of conditions.

Catalysis for Synthesis Sulfur-Organic Compounds

LIQUID-PHASE HYDROGENATION OF THIOPHENES ON PALLADIUM SULFIDE CATALYSTS

A.A. Zirka, A.V. Mashkina

Kinetics & Catalysis, 41 (2000) pp. 388-393.

Palladium sulfide catalysts are active for the hydrogenation of thiophenes of different structure in hydrocarbons at 220–300°C and 3.0–9.5 MPa. Thiophenes and benzothiophenes are close in reactivity. An increase in palladium sulfide concentration in the catalyst leads to an increase in the reaction rate per 1 g of the catalyst but has only a slight effect on the specific reaction rate of hydrogenation calculated per 1 g of Pd. The specific activity of palladium sulfide supported on aluminosilicate is one order of magnitude higher than that of PdS without a support and the catalysts supported on the aluminum oxide and carbon. The aluminosilicate-supported catalyst is also more selective.

ACTIVITY OF PALLADIUM SULFIDE CATALYSTS IN THE REACTION OF GAS-PHASE HYDROGENATION OF 2-METHYLTHIOPHENE

A.V. Mashkina, A.A. Zirka

Kinetics & Catalysis, 41 (2000) pp. 521-526.

In the interaction of hydrogen with 2-methylthiophene in the gas phase over palladium sulfide catalysts at 180–260°C and 0.1–0.8 MPa, the saturation of the thiophene ring resulting in 2-methylthiolane and the hydrogenolysis of 2-methylthiophene occurs. When the conversion is lower than 60%, these reactions occur independently; at higher conversions, methylthiolane also undergoes hydrogenolysis. The specific catalytic activity of PdS supported on ν-Al_2O_3, TiO_2, and carbon and without support is much lower in the hydrogenation of 2-methylthiophene than the activity of PdS supported on SiO_2, aluminosilicate, and zeolite HNaY having strong Brönsted acid surface sites.

EFFECT OF WATER ON HETEROGENEOUS CATALYTIC CONVERSION OF DIMETHYL DISULFIDE INTO METHANETHIOL

A.V. Mashkina, V.N. Yakovleva, L.G. Sakhaltueva

React. Kinet. & Catal. Lett., 70 (2000) pp. 183-189.

In dry helium at 350°C and 0.1 MPa, dimethyl disulfide is catalytically converted to yield methanethiol and products of elimination such as ethylene and H_2S. Methanethiol decomposes into H_2S and dimethyl sulfide in the presence of acid catalysts, and water introduced into the system hinders this process and provides an increase in the catalyst stability.

DIMETHYL DISULFIDE CATALYTIC CONVERSION INTO METHANETHIOL IN THE PRESENCE OF WATER

A.V. Mashkina

Kinetics & Catalysis, 41 (2000) pp. 216-221.

The processes of dimethyl disulfide conversion yielding methanethiol, ethylene and hydrogen sulfide, and the disproportionation of methanethiol formed in this reaction into hydrogen sulfide and dimethyl sulfide proceed on acid–base type catalysts at 350°C in the presence of water. Catalysts with weak proton sites exhibit low activity, which increases with the increasing surface acidity. Catalysts with weak Lewis acid sites and strong basic sites are most active and selective in the reaction of methanethiol formation. The presence of water inhibits the side reaction of disproportionation, thus enhancing the methanethiol formation selectivity.

Catalysis in Aqueous Solutions

IRON HYDROXIDES – NEW CATALYSTS FOR OXIDATION REACTIONS IN AQUEOUS SOLUTIONS

G.L. Elizarova, L.G. Matvienko, V.N. Parmon

Kinetics & Catalysis, 41 (2000) pp. 760-766.

The catalytic decomposition of H_2O_2 in the presence of SiO_2-supported amorphous and colloidal FeO(OH) is studied. An inactive Fe(IV) compound and a Fe(III) peroxo complex are found in the hydroxide composition. Possible mechanisms are discussed for H_2O_2 decomposition involving no free radicals. It is shown that lower hydrocarbons are oxidized in the systems, and their presence changes both the kinetics of H_2O_2 decomposition and the behavior of Fe(IV) and the peroxo complex.

THE ROLE OF PEROXO COMPLEXES IN THE CATALYTIC DECOMPOSITION OF H_2O_2 IN THE PRESENCE OF Cu(II) HYDROXIDES

G.L. Elizarova, L.G. Matvienko,
O.L. Ogorodnikova, V.N. Parmon

Kinetics & Catalysis, 41 (2000) pp. 323-339.

The catalytic decomposition of hydrogen peroxide is studied in the presence of colloidal and silica-gel-supported $Cu(OH)_2$. Copper peroxo complexes with different activities were identified. The reaction is molecular without radical formation. The mechanisms of H_2O_2 decomposition are discussed.

OXIDATION OF ORGANIC SUBSTANCES IN AQUEOUS SOLUTIONS OVER Ru CATALYSTS BY OXYGEN

M.V. Batygina, N.M. Dobrynkin, A.S. Noskov

Advances in Environmental Research J., 4 (2000) pp. 123-132.

The catalytic performance of supported Ru catalysts has been studied in the reactions of wet oxidation of acetonitrile, N,N-dimethyl formamide and carbamide at T=433-533 K and P=2.0-4.6 MPa, and wet oxidation of real sewage from an alcohol plant (so-called Luther water) at T=403-473 K and P=1.5-3.6 MPa. The Luther water contained a mixture of low-boiling (C_1-C_5) aldehydes and alcohols. The experiments were carried out in a perfectly mixed batch autoclave reactor. The conversion of alcohols and aldehydes contained in Luther water and selectivity of the process towards CO_2 and water as well as the selectivity of the oxidation of acetonitrile, N,N-dimethyl formamide and carbamide towards CO_2, N_2 and water were determined at various temperatures and reaction times. Ru (4.8 wt.%)/graphite-like carbon was effective in the oxidation of Luther water (ΔTOC=97.5% at T=423 K for 1h), carbamide ($X_{CO(NH2)2}$=100%, $S_{CO(NH2)2\rightarrow CO2}$=100%, $S_{CO(NH2)2\rightarrow N2}$=71% at 473 K, 2h) and acetonitrile (X_{CH3CN}=100%, $S_{CH3CN\rightarrow CO2}$=100%, $S_{CH3CN\rightarrow N2}$=75 % at 493 K, 1h). Ru/active carbon/γ-Al_2O_3 was effective in the oxidation of N,N-dimethyl formamide ($X_{HCON(CH3)2}$=100%, $S_{HCON(CH3)2\rightarrow CO2}$=61%, $S_{HCON(CH3)2\rightarrow N2}$=100% at 493 K).

CATALYTIC REDUCTION OF NITRATE AND NITRITE IONS BY HYDROGEN: INVESTIGATION OF THE REACTION MECHANISM OVER Pd AND Pd-Cu CATALYSTS

O.M. Il'initch, L.V. Nosova, V.V. Gorodetskii,
V.P. Ivanov, S.N. Trukhan, E.N. Gribov,
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J. Molec. Catal. A: Chemical, 158 (2000) pp. 237-249.

The catalytic behavior of mono- and bimetallic catalysts with Pd and/or Cu supported over γ-Al_2O_3 in the reduction of aqueous nitrate and nitrite ions by hydrogen was investigated. The composition of the supported metal catalysts was analyzed using secondary ion mass spectroscopy (SIMS) and X-ray diffraction (XRD) techniques. Surface enrichment of the bimetallic Pd-Cu particles in copper was revealed. Interactions of NO (possible intermediate in reduction of nitrate and nitrite ions) with H_2 over Pd were studied by thermal desorption spectroscopy (TDS) under high-vacuum conditions. The molecular mechanism of NO_3^- and NO_2^- reduction by H_2 as well as the role of Pd and Cu active sites are discussed.

CATALYTIC MEMBRANE IN REDUCTION OF AQUEOUS NITRATES: OPERATIONAL PRINCIPLES AND CATALYTIC PERFORMANCE

O.M. Il'initch, F.P. Cuperus*, L.V. Nosova,
E.N. Gribov (*Agrotechnological Research Institute, Wageningen, The Netherlands)

Catal. Today, 56 (2000) pp. 137-145.

The catalytic membrane with palladium–copper active component supported over the macroporous ceramic membrane, and a series of γ-Al_2O_3 supported Pd–Cu catalysts were prepared and investigated. In reduction of nitrate ions by hydrogen in water at ambient temperature, pronounced internal diffusion limitations of the reaction rate were observed for Pd-Cu/Al_2O_3 catalysts. The catalytic membrane with Pd–Cu active component deposited over the macroporous ceramic membrane support was employed to minimize the diffusion limitations. Multifold increase in the observed catalytic activity was registered for the catalytic membrane operated with the forced flow of the reaction solution through the membrane, as compared to the value achieved at the same conditions, but in the absence of the forced flow (i.e. when the membrane porous space was accessible to the reactants due to diffusion only). These improvements are attributed to the intensification of the intraporous mass transfer attainable with the reactants forced flow in the membrane pores.

The concept of catalytic membrane reactors explored in this study offers a new means to improve catalytic performance in the processes where internal diffusion limitations must be minimized and the use of finely dispersed catalysts is not desired.

CATALYTIC MEMBRANE IN DENITRIFICATION OF WATER: A MEANS TO FACILITATE INTRAPOROUS DIFFUSION OF REACTANTS

O.M. Il'initch, F.P. Cuperus*, R.W. van Gemert*, E.N. Gribov, L.V. Nosova (*Agrotechnological Research Institute, Wageningen, The Netherlands)

Separation & Purification Technology, 21 (2000) pp. 55-60.

The series of mono- and bi-metallic catalysts with Pd and/or Cu supported over γ-Al_2O_3 was investigated with respect to reduction of nitrate and nitrite ions in water by hydrogen. Pronounced limitations of catalytic performance due to intraporous diffusion of the reactants were observed in the reaction. Catalytic membrane containing the Pd–Cu active component supported over macroporous ceramic membrane-support was prepared, investigated and applied to facilitate the intraporous mass transfer. Forced flow of the reacting solution through the membrane was revealed to increase the effective catalytic activity. The approach explored in this study offers a cost-efficient alternative to the conventional concept of catalytic water denitrification process in a slurry reactor, presuming fixed-bed type operation with macroporous catalytic membranes at high level of catalytic activity.

Selective Water Sorbents and Heat Accumulating Materials

ADSORPTION PROPERTIES OF THE LITHIUM BROMIDE-WATER SYSTEM IN PORES OF EXTENDED GRAPHITE, SIBUNIT, AND ALUMINA

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Russ. J. Phys. Chem., 74 (2000) pp. 2016-2020.

The sorption equilibrium of lithium bromide dispersed in pores of ν-alumina, a synthetic carbon material (extended graphite and Sibunit) with water vapor, was studied by thermogravimetry over the temperature range from 30 to 135°C at a water vapor pressure of P_{H2O}=6.0–81.0 mbar. It was established that the main characteristics of the sorption equilibrium under study are determined by the dispersion characteristics of the salt rather than by the chemical nature of the matrix. For matrices with an average pore diameter larger than 15 nm, the sorption at small relative pressures of water vapor is monovariant and results in the formation of the $LiBr \cdot H_2O$ crystal monohydrate; a further sorption is accompanied by the formation of an aqueous solution of the salt, and the equilibrium becomes bivariant. The sorption properties of crystal hydrates and solutions formed in such pores are similar to those of the $LiBr$-H_2O bulk system. For LiBr dispersed in pores with an average diameter smaller than 8 nm, the sorption equilibrium is bivariant in the entire range of sorption values, which means that no crystal hydrate is formed in such pores. A comparison with the $LiBr$–H_2O bulk system shows that the sorption capacity of the dispersed salt increases in the range of existence of the bulk crystal hydrate and decreases in the range of existence of the solution. The isosteric heats of sorption of water vapor were determined.

SELECTIVE WATER SORBENTS FOR MULTIPLE APPLICATIONS.
10. ENERGY STORAGE ABILITY

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React. Kinet. & Catal. Lett., 69 (2000) pp. 345-354.

Energy storage ability E is measured over $T = 50\text{-}340^{o}C$ for more than fifteen samples of selective water sorbents based on silica gels, aluminas, carbon Sibunit and aerogels as host matrices and $CaCl_2$, LiBr, $MgCl_2$ as impregnated salts. The E-values up to 8.4 kJ/g and 4.0 kJ/g are found for forced and naturally saturated sorbents, that are much higher than for common materials. These values make the sorbents promising for long-term energy storage. The temperature dependence of E gives an estimation of sensible and latent heat contributions as well as the specific heat of a dry sorbent. The relation between the energy storage ability and water content allows to obtain the heat of water desorption and can be used for brief estimation of energy storage ability for a variety of SWS composites. A comparison between the SWS materials and other proposed in literature is done.

SELECTIVE WATER SORBENTS FOR MULTIPLE APPLICATIONS.
11. $CaCl_2$ CONFINED TO EXPANDED VERMICULITE

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React. Kinet. & Catal. Lett., 71 (2000) pp. 377-384.

This paper presents sorption properties of new selective water sorbent based on the vermiculite as a host matrix and calcium chloride as a hygroscopic salt. Sorption isobars, isosters and isotherms at T=30-150°C and vapor partial pressure 10-31 mbar clearly showed that at low water contents crystalline hydrates with 0.33 and 1 molecule of water per 1 molecule of $CaCl_2$ are formed. These hydrates are stable over a temperature range of 20-30°C and posses kinetically slow transformations. The stabilizing effect of vermiculite matrix is discussed. At higher water contents the vapor absorption leads to the formation of the salt solution inside pores. The solution properties can be described by the Dubinin-Astakhov equation and are close to those known from literature for the bulk solutions. Isosteric sorption heat is measured to depend on water sorption and to change from 75.5 kJ/mol for solid hydrates to 42.2-45.6 kJ/mol. for solution.

CONCENTRATED AQUEOUS ELECTROLYTE SOLUTIONS: ANALYTICAL EQUATIONS FOR "HUMIDITY-CONCENTRATION" DEPENDENCE

S.I. Prokopiev, Yu.I. Aristov

J. Solut. Chem., 29 (2000) pp. 633-649.

In this paper analytical equations of Henry, Freundlich, Dubinin-Astakhov, Brunauer-Emmett-Teller and a new modification of the BET equation are used for thermodynamic description of water activity over wide temperature (260-600 K) and water mole fraction (0.3-0.8) ranges for concentrated aqueous solutions of electrolytes. The solutes considered are H_2SO_4, $CaCl_2$, LiBr, LiCl, LiI, $MgCl_2$ and NaOH in bulk state and $CaCl_2$, LiBr in dispersed state. The generalized Henry equation is found to allow a correct extrapolation of the bulk solution properties measured at low and moderate salt concentrations to the region of low water contents. The suggested modification of the BET equation as well as the Dubinin-Astakhov equation give a precise (with a relative error less than 1 %) description of literature data on the "humidity-concentration" dependence and can be used for the reliable prediction of this dependence in the region of intermediate conditions.

THERMAL CONDUCTIVITY OF A SILICA GEL + CALCIUM CHLORIDE SYSTEM: THE EFFECT OF ADSORBED WATER

Yu.Yu. Tanashev, Yu.I. Aristov

J. Engin. Physics & Thermophysics, 73 (2000) pp. 876-883.

An effecient coefficient of heat conductivity λ of the system “silica gel KSK + calcium chloride” has been measured by the “hot wire” method at T=293 K. It is found that the heat conductivity gradually increases with the raise of the water uptake *w*. The sharp increase in λ is observed when a continuous phase of aqueous salt solution is formed inside the silica pores. The results obtained are satisfactorily described by Luikov-Bjurstrom model.

SORPTION OF CARBON DIOXIDE FROM WET GASES BY K_2CO_3-IN-POROUS MATRIX: INFLUENCE OF THE MATRIX NATURE

A.G. Okunev, V.E. Sharonov, Yu.I. Aristov, V.N. Parmon

React. Kinet. & Catal. Lett., 71 (2000) pp. 355-362.

In a fixed-bed absorber at 40°C, the dynamics of carbon dioxide sorption over composite sorbents prepared by impregnation of potassium carbonate in various porous matrixes is studied. The dynamic capacity of the synthesized sorbents is shown to reach 0.12 g CO_2 per 1 g of the sorbent. The composite dynamic capacity depends on the nature of the host matrix and decreases in the sequence alumina>activated carbon>silica gel. For K_2CO_3-on-alumina, the sorption capacity decreases considerably after the first cycle of "absorption and regeneration under 200-350°C", whereas the sorbents based on active carbons could be reversibly restored. The findings are discussed within the idea of a chemical interaction between the host matrix and the impregnated salt.

Catalysis and Biotechnology

SYNTHESIS OF THE SCALEMIC ALKALOID (-)-DIPTHOCARPAMINE

N.N. Karpyshev, A.G. Tolstikov, O.V. Tolstikova, O.D. Yakovleva, V.S. Shmakov

Russ. Chem. Bull., 49 (2000) pp. 564-565.

The synthesis of scalemic forms of active Alkaloid (-)-Dipthocarpamine has been carried out by asymmetric oxidation of N-isopropyl-N'-methylthiohexyl urea with hydrogen peroxide in the presence of vanadium (IV) complexes with chiral shiff bases.

SYNTHESIS OF (-)-α-METHYLDESMOTROPSANTONINE NITROGEN-CONTAINING DERIVATIVES

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(*Institute Of Organic Chemistry, Novosibirsk, Russia)

Russ. J. Org. Chem., 36 (2000) pp. 93-98.

The transformations of (-)-α-methyldesmotropsantonine into tetrahydronaphtalene series hydrazides and amines have been studied. The latest compounds applicability in synthesis of chiral picoline- and salicylaldimines have been investigated.

SYNTHESIS OF 1-ETHYLPYRROLIDONE-2 BY HYDROGENATION OF 1-VINYLPYRROLIDONE-2 OVER A Pd/C CATALYST

I.L. Simakova, V.A. Semikolenov

Kinetics & Catalysis, 41 (2000) pp. 383-387.

A selective catalytic system for the hydrogenation of 1-vinylpyrrolidone-2 (VP) to 1-ethylpyrrolidone-2 (EP) is found. The factors responsible for the formation of by-products in the conversion of VP are studied. The presence of acid sites or radical species in a catalytic system results in the fast polymerization of VP.

The resulting by-product, polyvinylpyrrolidone, may deactivate the hydrogenation catalyst by surface blocking.

VP can be hydrogenated to EP under mild conditions and with a high selectivity using a palladium catalyst supported on a porous carbon material Sibunit. The kinetics of VP hydrogenation over the Pd/C catalyst is studied.

ADSORPTION OF ANTISEPTICS (FURACILLIN, CHLOROHEXYDINE) AND VITAMIN E ON CARBON CONTAINING ENTEROSORBENTS

G.A. Kovalenko, E.V. Kuznetsova

Chemical-Pharmaceutical J., 34 (2000) pp. 45-49.

Adsorption properties of carbon containing enterosorbents of SUMS-1, Polyphepan and Carbactine types with respect to anticeptics (Furacillin, Chlorohexydine) and vitamin E (α-tocopherol) were studied to develop medicine of prolonged action with local therapeutic effect.

The Carbactine was shown to possess maximum adsorption capacity to Furacillin and Vitamin E (~200 mg/g), SUMS-1 – to Chlorohexydine (~ 400 mg/g). At the same time adsorption capacity of Polyphepan to biologically active substances under consideration was close to zero. The surface of the biologically active substances of different molecular weight available for adsorption of enterosorbents was shown to be determinative.

Catalysis for Detoxication

A ROLE OF CATALYSIS FOR THE DESTRUCTION OF WASTES FROM THE NUCLEAR INDUSTRY

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Catal. Today, 55 (2000) pp. 23-43.

Recent advances in application of catalysis to problems of waste destruction and off-gas treatment in the nuclear industry are presented: destruction of mixed organic wastes in a fluidized catalyst bed, mixed waste oxidation in catalytically active molten salts, selective catalytic reduction of NO_x, in off-gases, catalytic oxidation of H_2 in the ventilation exhaust from liquid waste tanks and catalytic removal of VOCs in processes of groundwater and soil remediation.

OXIDATION OF ORGANIC COMPOUNDS AND CARBON MONOXIDE IN SOME MOLTEN SALTS AND CATALYSTS. ADVANCES IN MOLTEN SALTS. FROM STRUCTURAL ASPECTS TO WASTE PROCESSING

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Proceedings of the European Research Conference on Molten Salts,
Editor M. Gaune-Escard, New York, 1999, pp. 279-299.

The study of the performance of some molten salt systems in oxidation of organic compounds and CO was carried out with special emphasis on the effect of catalytically active additives on the oxidation efficiency.

The destruction of various organic compounds, such as methane, propane, chlorobenzene, carbon tetrachloride and CO was studied in the melts: NaOH-KOH; LiCl-KCl, Li_2SO_4-Na_2SO_4, Li_2CO_3-K_2CO_3; carbonates doped with transition metal oxides (Fe_2O_3, Cr_2O_3, Co_3O_4, MnO_2) and catalytically active K_2O-V_2O_5 system (pure and doped with CuO).

The effects of melt composition, oxygen concentration, load on melt, and temperature on destruction efficiency were studied.

The experimental results have shown that molten catalysts based on V_2O_5 or alkaline metal carbonates can be effectively used for the oxidation of CO and organic compounds.

Catalyst performance depends on its composition and operation conditions. Addition of oxides of transition metals (Fe, Cr, Mn, Co, Cu) is observed to increase the efficiency of destruction.

DEVELOPMENT OF CATALYTIC TECHNOLOGIES FOR PURIFICATION OF GASES FROM HYDROGEN SULFIDE BASED ON DIRECT SELECTIVE OXIDATION OF H_2S TO ELEMENTAL SULFUR

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Eurasian Chem. Tech. J., 1 (1999) pp. 49-56.

In the Boreskov Institute of Catalysis in cooperation with specialists of All-Russian Institute of Hydrocarbon Raw Materials novel methods of purification of fossil fuels based on oxidation of hydrogen sulfide to elemental sulfur have been developed. In this paper the results of laboratory and pilot plant testing of the technologies are presented.

CATALYTIC SYSTEMS PROMOTE THE SOLUTION OF ECOLOGICAL PROBLEMS

V.N. Romannikov

Chemistry and Business, 35 (1999) pp. 64.

The main technological characteristics of the catalysts based on high-silica zeolites for the process of benzene alkylation by ethylene developed at Boreskov Institute of Catalysis are considered.

KINETICS AND MECHANISM OF LOW-TEMPERATURE OXIDATION OF H_2S WITH OXYGEN IN THE GAS PHASE

O.N. Kovalenko, N.N. Kundo, P.N. Kalinkin

React. Kinet. & Catal. Lett., 7 (2000) pp. 139-145.

The possibility of the formation of polysulfides during oxidation of H_2S with oxygen on oxide catalysts has been checked, and the sequence of the reaction stages at temperatures below the sulfur dew point determined. The amount of polysulfides formed during H_2S oxidation has been found to exceed significantly that obtained in the reaction of sulfur with H_2S. Polysulfides are concluded to be intermediates in H_2S oxidation to sulfur. The rate of formation of SO_2 from sulfur vapor is shown to be negligibly low at 100-200°C. A reaction scheme involving the formation of sulfur from polysulfides and the formation of sulfur dioxide by direct oxidation of H_2S is suggested.

SELECTIVE OXIDATION OF HYDROGEN SULFIDE IN THE FLUIDIZED CATALYST BED REACTOR IN THE CASE OF SULFUR CONDENSATION AND CATALYST CIRCULATION

G.G. Kuvshinov, S.G. Zavarukhin, M.Yu. Lebedev, D.G. Kuvshinov, S.V. Vanag* (*Novosibirsk State Technological University, Novosibirsk, Russia)

Scientific Bull. of NSTU, 2 (1999) pp. 135-150.

The possibility of purification of gases from hydrogen sulfide during its selective oxidation at elevated pressures under conditions of formation of condensed sulfur on the catalyst has been analyzed. A flow sheet for the process of hydrogen sulfide oxidation in a fluidized catalyst bed reactor in the case of sulfur condensation and catalyst circulation has been suggested, and a mathematical model for the process performed in the reactor under the steady-state conditions has been developed. The model bases on the two-phase fluidized bed approximation allowing for the catalyst particle distribution with respect to sulfur content, dependence between the catalyst activity and sulfur concentration, and mass exchange between dense and bubble phases, and assuming the plug regime by the bubble phase and the ideal mixing regime by the dense phase. The model allowed to calculate the process parameters as the function of regime parameters.

PROCESS COUPLING AS A WAY TO IMITATION OF NATURAL WASTELESS TECHNOLOGY

G.I. Panov

Chemistry for Sustainable Devel., 8 (2000) pp. 547-553.

The method preferably used now for environmental protection from hazardous chemical wastes is based on pre-neutralization of the wastes, *i.e.* their transformation into less ecologically harmful compounds. However, the rapidly increase amount of wastes, even if neutralized, makes a serious danger to the environment. The nature prompts to us a higher-order solution, *viz.* design of coupled technologies implying the used of wastes from one process as feedstock for another one. This is exactly the approach underlying integration of all the innumerable chemical transformations, which occur in the living nature, into the global nonwaste technology. The very term “wastes” is inapplicable to natural technologies. One of the earliest attempts of application of such an approach to catalytic chemistry is discussed in the present paper. This is an example of development of new oxidation processes based on unique oxidative behavior of nitrogen suboxide wasted at the production of adipic acid.

Catalytic Technologies for Combustion

A CATALYTIC METHOD FOR PRODUCING HEAT FROM LOW-HEATING-VALUE GASES

O.P. Klenov, L.L. Gogin, A.S. Noskov

Thermal Engineering, 47 (2000) pp. 928-932.

Results of the development and experimental validation of the technology for producing high potential heat from air mixtures with a low content of different kinds of fuel, such as organic compounds, hydrogen, and carbon monoxide, are presented. The proposed technology employs flameless catalytic combustion of fuel under conditions of the so-called reverse process, that is, periodically changing the direction of flow of the fuel passing through an immobile layer of catalyst particles.

STUDY OF THE CATALYSTS FOR FUEL COMBUSTION REACTIONS: 19. THERMAL STABILITY OF ALUMINA PROMOTED WITH LANTHANUM AND SILICON

R.A. Shkrabina, V.A. Ushakov, N.A. Koryabkina, Z.R. Ismagilov

Kinetics & Catalysis, 41 (2000) pp. 394-398.

X-ray diffraction analysis and data on the strength and specific surface area are used to study the thermal stability of a La–Si/Al_2O_3 system depending on the concentration of introduced additives and calcination temperature. The mechanisms of interactions of these elements and alumina are discussed.

Silicon and lanthanum cations begin to interact at low temperatures (~500°C). The authors assume that silicon and lanthanum cations occupy tetrahedral and octahedral positions, respectively, in the ν-alumina lattice and thus significantly enhance its thermal stability. Up to 50% of ν-Al_2O_3 is retained at 1200°C, and α-Al_2O_3 starts to form in the ternary system only at 1300°C.

STUDY OF THE CATALYSTS FOR FUEL COMBUSTION REACTIONS: 20. THERMAL STABILITY AND OTHER PROPERTIES OF THE $CeO_2 \cdot MgO \cdot Al_2O_3$ SYSTEM

N.A. Koryabkina, R.A. Shkrabina, V.A. Ushakov, Z.R. Ismagilov

Kinetics & Catalysis, 41 (2000) pp. 662-669.

The effect of simultaneous addition of magnesium and cerium cations on the structure formation and properties of aluminum oxide obtained from hydroxides with different phase compositions by thermal treatment at 773–1573 K is studied. At temperatures lower than 1273 K, the effect of specific surface area stabilization is observed for the samples. It is found that spherical aluminum oxide modified with Mg and Ce cations exhibits high mechanical strength upon calcination at T>1373 K. Modified samples calcined at 1573 K are catalytically active in the CH_4 oxidation reaction.

NEW DATA ON GAS-PHASE RADICAL REACTIONS IN THE STEAM REFORMING OF METHANE IN THE PRESENCE OF CATALYSTS. 1. NICKEL CATALYSTS

I.I. Bobrova, V.V. Chesnokov, N.N. Bobrov, V.I. Zaikovskii, V.N. Parmon

Kinetics & Catalysis, 41 (2000) pp. 19-24.

Methane pyrolysis and steam reforming were studied over a series of nickel catalysts ($Ni-Al_2O_3$, Ni/MgO, and $Ni/LiAlO_2$) under the same conditions (650-750°C, P_{CH4}=0.001-0.03 MPa). Unlike heterogeneous reaction of pyrolysis, some of the steps of steam reforming of methane occur in the gas phase. When gas-phase reactions were suppressed, the rate and activation energy of steam reforming were close to the corresponding kinetic characteristics for pyrolysis. Hypothetically, the rate-limiting step of the process is the dissociative adsorption of methane on nickel in this case.

Pt AND Pd SUPPORTED ON GLASS FIBERS AS EFFECTIVE COMBUSTION CATALYSTS

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Catal. Today, 59 (2000) pp. 61-68.

Pd and Pt supported on the glass fibers with a developed surface and high specific surface have been studied in the complete propane oxidation. The reaction was carried out in a circulating reactor and kinetic parameters were estimated under various reaction conditions in the temperature range of 200-500°C. Pt catalysts have been shown to be more active than Pd ones with the same metal content on the identical support. The catalytic activity has been shown to depend on the support composition. The most high activity is exhibited on Pt supported on the glass fibres modified by titanium oxide with the ignition temperature of about 200°C. The surface morphology and surface distribution of the active component were described by the high resolution electron microscopy.

Liquid-Phase Catalytic Technologies

KINETIC STUDY OF LIQUID-PHASE HYDRODECHLORINATION OF HEXACHLOROBENZENE ON Ni/C AND 2%PdNi/C

V.A. Yakovlev, V.I. Simagina, S.N. Trukhan, V.A. Likholobov

Kinetics & Catalysis, 41 (2000) pp. 25-32.

Liquid-phase hydrodechlorination of hexachlorobenzene was kinetically studied in the presence of both nickel (Ni/C) and palladium-promoted nickel (2%PdNi/C) catalysts under different reaction conditions. Molecular hydrogen (at 1 and 20 atm) and sodium borohydride ($NaBH_4$) were used as reducing agents. In the presence of the nickel catalyst, the hydrodechlorination of C_6Cl_6 occurs via a consecutive mechanism (removal of one chlorine atom from the substrate at each stage), whereas with the 2%PdNi/C catalyst, the transformation of C_6Cl_6 occurs via both consecutive and multiplet mechanism (with the elimination of several chlorine atoms without desorption of the chloroaromatic substrate from the catalyst surface). The promotion of the nickel catalysts with palladium substantially changes the selectivity of formation of intermediate products of C_6Cl_6

dechlorination. The mechanism of hydrodechlorination of hexachlorobenzene was suggested that explained the presence of only certain products of partial dechlorination of hexachlorobenzene in the reaction medium.

LIQUID PHASE CATALYTIC HYDRODECHLORINATION OF CHLOROBENZENE OVER SUPPORTED NICKEL AND PALLADIUM CATALYSTS: AN NMR INSIGHT INTO SOLVENT FUNCTION

V.A. Yakovlev, V.V. Terskikh, V.I. Simagina, V.A. Likholobov

J. Molec. Catal. A: Chemical, 153 (2000) pp. 231-236.

The catalytic hydrodechlorination of chlorobenzene with Ni/C, Pd/C and $Ni_{98}Pd_2/C$ in ethanol was studied with ^{3}D and ^{13}C {^{1}H} NMR. Two dechlorination routes of this reaction (ionic and free-radical) are suggested depending upon the nature of the active hydrogen species. At the same time two competitive sources of hydrogen for hydrogenolysis of the C-Cl bond molecular hydrogen and solvent (ethanol) molecules - are readily apparent from experiments with molecular deuterium.

NEW DOMESTIC CATALYTIC TECHNOLOGIES TO SAVE ENERGY AND RESOURCES AND TO PROTECT ENVIRONMENT

A.S. Noskov, V.N. Parmon

Chemical Industry, 1 (2000) pp. 28-33.

In the article there is given a survey of catalytic technologies developed at the Boreskov Institute of Catalysis and designated for the reduction of material (power) expenditures in the chemical processes. Particular emphasis has been paid to the catalytic methods of incineration of substandard fuels and processes of purification of sewage by the method of liquid phase catalytic oxidation.

CARBOXY DERIVATIVES OF COBALT PHTHALOCYANINE IN LIQUID-PHASE OXIDATION OF HYDROGEN SULFIDE BY OXYGEN IN THE PRESENCE OF CYANIDE IONS

G.A. Faddeenkova, N.A. Drugova*, V.E. Maizlish*, G.P. Shaposhnikov*, N.N. Kundo (*Ivanovo State University of Chemical Technology, Ivanovo, Russia)

Russ. J. Appl. Chem., 73 (2000) pp. 820-823.

The effect of the structure of various tetra- and octacarboxy derivatives of cobalt phthalocyanine on their catalytic activity in liquid-phase oxidation of hydrogen sulfide with oxygen in the presence of cyanide ions was studied.

Nucleation Processes

N-PENTANOL–HELIUM HOMOGENEOUS NUCLEATION RATES

M.P. Anisimov, P.K. Hopke*, S.D. Shandakov, I.I. Shvets (*Clarkson University, Potsdam, New York, USA)

J. Chem. Phys., 113 (2000) pp. 1971-1975.

An international collaboration to examine the effects of different experimental systems on nucleation measurements has resulted in a series of nucleation experiments on the *n*-pentanol–helium system. In particular, using a laminar flow diffusion chamber, nucleation rate data were obtained for temperatures between 258 and 266 K and total pressures of 0.10, 0.20, and 0.30 MPa. These results are compared with other data on nucleation measured experimentally using an expansion wave tube, a two-piston expansion chamber, a flow diffusion chamber, and a static diffusion chamber. The influence of the carrier gas pressure on nucleation rates was explored. It was concluded that the critical embryo phase transitions should be detectable in an analogous manner to the recently reported phase transitions in the glycerin–carbon dioxide system. The experimental detection of the melting point is suggested as a critical test for the ability of an experimental system to provide adequate measurements of nucleation rates. For example, the glycerin melting point can be used for these tests. A reference equation for nucleation rates of *n*-pentanol–helium is proposed as a practical test of any experimental measurement system for total pressures of 0.10, 0.20, and 0.30 MPa. The use of this equation is recommended even if the reference equation is not completely accurate, because it provides a scale for comparison of the results for different research groups and methods.

EXPERIMENTAL DETECTION OF NUCLEATION RATE SURFACE SINGULARITY

M.P. Anisimov, A.G. Nasibulin, S.D. Shandakov

J. Chem. Phys., 112 (2000) pp. 2348-2354.

As a rule, the modern theories of nucleation represent only modifications of classical theory, and they still remain unsuitable for quantitative prediction of experimental results. In order to create the universal description of supersaturated vapor nucleation, as well as evaluate other theories, it is necessary to get the reliable experimental results. Now experimental skills are high enough for precision measurements of the vapor nucleation rates as well as for detecting and evaluating, for example, temperatures of phase transitions in the new phase critical embryos. That is, one can find experimentally the singularity of the nucleation rate surface at conditions for the critical embryo phase transitions. Visual analysis of the experimental results has the low potential to detect the nucleation rate surface singularity and the surface singularity can be missed sometimes. One major problem for singularity detection is the noise of experimental results. This problem still exists even if one has experimental results of high accuracy. The condition for surface continuity and monotony could be applied as a criterion for analysis of experimental data for the vapor nucleation rates. The criterion is tested for the broad spectrum of the experimental results in the vapor nucleation. As an example of the criterion being used, the experimental results for the *n*-pentanol–water binary system of nucleation have been analyzed. A peculiarity of this system is the existence of a miscibility gap between the components. It was found that the criterion as a function of *n*-pentanol mole fraction has the singularity in the vicinity of this gap. This singularity was smoothed in the experimental results presentation and omitted in the original research. The proposed criterion can be used to search the experimental data set singularity as a function of their variable(s).

POTENTIAL WAYS TO STUDYING FREQUENCIES FOR DESTRUCTION AND FORMATION OF METHANE HYDRATE NUCLEI

M.P. Anisimov, S.D. Shandakov, A.G. Nasibulin, Yu.I. Polygalov

Chem. for Sustainable Devel., 8 (2000) pp. 465-475.

Possibility to assess boundaries of undangerous metastability of gaseous hydrates is discussed in terms of the nucleation theory. Theoretical and experimental state of the art is analyzed and potential schemes were proposed for experiments with gaseous hydrates.

1,2-PROPANEDIOL AND 1,3-PROPANEDIOL HOMOGENEOUS NUCLEATION RATES AND PHASE TRANSITIONS IN THE NEW PHASE CRITICAL EMBRYOS

M.P. Anisimov, J.A. Koropchak*, A.G. Nasibulin, L.V. Timoshina (*Southern Illinois University, Carbondale, Illinois, USA)

J. Chem. Phys., 112 (2000) pp. 9917-0028.

Nucleation rates of supersaturated vapors near the conditions for the critical line for each pair of 1,2- or 1,3-propanediol and carbon dioxide or sulfur hexafluoride at total system pressures of P = 0.10, 0.20, and 0.30 MPa have been measured in a flow diffusion chamber. Critical parameters, i.e., temperatures and pressures, of the binary systems versus compositions were semiempirically evaluated. It was found experimentally that there is an area of parameters in the *PTx* phase diagram, for each pair of vapor and carrier gas investigated in the present research, for which critical embryo phase transitions of the first order take place (where P, T, and x are pressure, temperature, and embryo composition, respectively). The nucleation rate surface singularity and a gap in the number of molecules in critical embryos reflect this area. Shifts of the phase transition temperatures can be initiated by increasing the pressure (or concentration) of the carrier gas. This behavior is peculiar for binary systems. It is well-known that no liquid–liquid phase transitions can exist for a one-component system. At least a binary solution is required for liquid–liquid phase transitions. This means that vapor nucleation of the investigated substances in the carrier gas atmosphere can be considered as nucleation of a binary vapor–gas system. A schematic diagram for the possible metastable vapor conditions is presented. On the basis of our experimental results, one can assume that there exists a surface describing the parameters related with a phase transition of the first order in critical embryos. This surface is located within the volume of the possible vapor metastable conditions.

Mathematical Simulation of the Processes and Reactors. Chemical Engineering

SUPERCRITICAL FISCHER-TROPSCH SYNTHESIS: THE EFFECT OF NONIDEALITY OF THE REACTION MIXTURE ON THE REACTION RATE

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(*Laboratory of Petrochemical Technology,
University of Gent, Gent, Belgium)

Theor. Found. of Chem. Engin., 34 (2000) pp. 180-188.

A kinetic model is derived from experimental data for the Fischer–Tropsch reaction on a precipitated iron catalyst. In this model, the effect of nonideality of the reaction medium on the reaction rate is taken into account by introducing fugacity coefficients derived from a modified Redlich–Kwong–Soave equation of state. Coefficients of the Schulz–Flory distribution for saturated and unsaturated hydrocarbon products were calculated as functions of CO and H_2 fugacities in the reaction mixture. The proposed kinetic model is applicable at T = 523–623 K and P = 6–100 atm. A method based on the calculated critical parameters of the reaction mixture is proposed for the selection of suitable supercritical solvent and for the optimization of its concentration. The reaction rate and the total yield of C_nH_{2n} ($n \geq 2$) olefins (including the desired fraction C_5-C_{11}) under supercritical conditions were demonstrated to be essentially higher than those for the reference process carried out in the absence of solvent.

THERMODYNAMIC CALCULATIONS IN MODELING OF MULTIPHASE PROCESSES AND REACTORS

A. Yermakova, V.I. Anikeev

Ind. Eng. Chem. Res., 39 (2000) pp. 1453-1472.

A two-parameter cubic Soave-Redlich-Kwong equestion of state with modified binary interaction coefficients has been used for phase equilibrium calculations of multicomponent systems under supercritical and near-critical conditions. Example calculations of the phase behavior of multicomponent reaction mixture are presented and used to illustrate the increased accuracy of the SRK equation of state with the new binary interaction coefficients. The homotopy continuation method was adapted for the solution of the model equations by using temperature and pressure as continuation parameters. The effective models and algorithms thus created are used for the phase state calculations, localization of the critical point of multicomponent mixtures, studies of phase properties near the critical point, and determination of parameter regions that are of practical importance for the process performance under supercritical conditions. The problems of existence and uniqueness of a solution are studied. A new method for solving equations for the critical phase is suggested. Many examples of the calculation of phase diagrams of mixtures with a supercritical solvent are presented and the results compared with the reference data.

CALCULATION OF SPINODAL LINE AND CRITICAL POINT OF A MIXTURE

A. Yermakova, V.I. Anikeev

Theor. Found. of Chem. Engin., 34 (2000) pp. 51-58.

A simple form of two equations that describe the spinodal line on the T–P plane and the critical point of a multicomponent mixture is suggested. This form is easy to implement numerically. An effective solution algorithm for model equations that is based on the parameter continuation method is proposed. Results of computation are compared with the literature data obtained from other models, as well as with experiments. An example of parameter calculation for benzene hydrogenation in supercritical CO_2 is given.

CATALYTIC TECHNOLOGIES OF THE FUTURE FOR RENEWABLE AND NON-TRADITIONAL ENERGETICS

V.N.Parmon

Chemistry for Sustainable Devel., 8 (2000) pp. 555-565.

Modern trends in development of new catalytic technologies for employing nuclear, non-traditional and renewable energy sources, for generation of mechanical and electric energy from the energy of chemical cells, as well as for accumulation and utilization of moderate- or low-potential heat wastes and temperature gradients are overviewed.

THERMODYNAMIC EQUILIBRIUM IN THE SYNTHESIS OF DIMETHYL ETHER FROM SYNTHESIS GAS

V.D. Meshcheryakov, V.A. Kirillov

Theor. Found. of Chem. Engin., 34 (2000) pp. 85-89.

Chemical equilibrium in dimethyl ether synthesis from synthesis gas was studied thermodynamically over wide ranges of gas compositions and process parameters.

EFFECTS OF THE ACTIVE COMPONENT DISTRIBUTION IN A CATALYST PARTICLE ON THE POLYMER PRODUCT MORPHOLOGY

V.B. Skomorokhov, V.A. Zakharov, V.A. Kirillov

Polymer Science, Ser. A, 42 (2000) pp. 1163-1168.

The results of mathematical modeling of the catalytic polymerization of ethylene, performed within the framework of a multiparticle model, showed that morphology of the final polyethylene (PE) particles may be significantly affected by inhomogeneity of the initial active component distribution in the catalyst particles. It was found that, in contrast to the existing notions according to which the catalyst particle structure uniquely determines the final structure of polymer grains, the local changes in concentration of the active component may lead to the appearance of both loose (voids) and dense regions in the local polymer structure. It was also established that retarded internal diffusion of the monomer may lead to a decrease in density of the internal regions of PE grains and, eventually, in the polymer powder density.

EXTERNAL DIFFUSION CONTROL IN THE GAS-PHASE DEHYDROGENATION OF HYDROCARBONS ON A CATALYST PELLET

V.A. Kirillov, N.A. Kuzin, A.V. Kulikov,
B.N. Luk'yanov, V.M. Khanaev, A.B. Shigarov

Theor. Found. of Chem. Engin., 34 (2000) pp. 475-484.

External-diffusion gas-phase mass transfer in the catalytic hydrogenation of hydrocarbons was studied theoretically and experimentally. For the model of a stationary diffusion film around a catalyst pellet, an approximate solution of Maxwell–Stefan equations was obtained, which allowed the multicomponent diffusion problem to be reduced to a Fick equation involving a pseudobinary effective diffusion coefficient. A comparison was made between the theoretical and experimental results for the hydrogenation of α-methylstyrene, octene, and their mixtures.

HYDROGEN PRODUCTION BY STEAM REFORMING OF ETHANOL: A TWO STEP PROCESS

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G. Cacciola*, V.N. Parmon, V.A. Sobyanin
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React. Kinet. & Catal. Lett, 71 (2000) pp. 143-152.

A two-layer fixed-bed catalytic reactor for hydrogen production by steam reforming of ethanol has been proposed. In this reactor ethanol is firstly converted to acetaldehyde over Cu-based catalyst and then acetaldehyde is converted to hydrogen-rich mixture over Ni-based catalyst. It has been shown that the use of such type reactor prevents coke formation and provides hydrogen yield closed to equilibrium

DEVELOPMENT AND STUDY OF METAL FOAM HEAT-EXCHANGING TUBULAR REACTOR: CATALYTIC COMBUSTION OF METHANE COMBINED WITH METHANE STEAM REFORMING

Z.R. Ismagilov, O.Yu. Podyacheva,
V.V. Pushkarev, N.A. Koryabkina,
V.N. Antsiferov*, Yu.V. Danchenko*,
O.P. Solonenko, H. Veringa***** (*Republic Center of Powder Metallurgy, Perm, Russia; **Institute of Theoretical and Applied Mechanics, Novosibirsk, Russia; ***ECN, ZG Petten, The Netherlands)

Stud. Surf. Sci. & Catal.,
Proceedings of the 12th International Congress on Catalysis,
130 (2000) pp. 2759-2764.

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 rector 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.

MODELING OF n-BUTANE OXIDATIVE DEHYDROGENATION IN A DUAL-REACTOR SYSTEM

S.I. Reshetnikov, N.M. Ostrovskii

React. Kinet. & Catal. Lett., 71 (2000) pp. 129-136.

A mathematical modeling of the oxidative dehydrogenation of n-butane into butadiene in a dual-reactor system with the separate reactants feeding has been performed. The factors effected on the butadiene selectivity enhancement has been studied. It has been shown that it is possible to regulate the state of a catalyst in the reaction zone by varying the rate of the catalyst circulation.

INDUSTRIAL EXPERIENCE OF HEAT SUPPLY BY CATALYTIC INSTALLATIONS

A.D. Simonov, N.A. Yazykov, P.I. Vedyakin,
G.A. Lavrov, V.N. Parmon

Catal. Today, 60 (2000) pp 139-145.

A new technology of fuel combustion, offered by the Boreskov Institute of Catalysis in industrial scale, allows avoiding many disadvantages of the high-temperature fuel combustion. The technology is based on a combination of four principles: use of heterogeneous catalysts for complete oxidation of combustibles; combustion of fuels in a fluidized bed of catalyst particles; combustion of fuels without a significant excess of air; overlapping the processes of heat release and removal within the same fluidized bed. Basing on the new technology, a variety of apparatuses for the liquids heating and evaporation, for materials drying and heating, for detoxification of industrial emissions (gaseous, liquid, and solid), and for a number of other processes have been designed. Pilot catalytic heat supply units (CHSU) have being used since the early 1980s to heat the auxiliary and constructed buildings. Since 1993 30 industrial CHSUs operate successfully and reliably at different facilities in the Novosibirsk Province, Russia; all working parameters correspond to the design values. Automatic feedback between the temperature of circulating water and fuel feed allows minimizing the fuel consumption, in regard to the heat yield and temperature of the outside air. The content of toxic substances in the CHSU flue gases does not exceed sanitary norms. An important advantage of catalytic combustion in the fluidized catalyst bed is the opportunity to burn efficiently the solid fuels (coal, peat) as well.

INVESTIGATION OF THE MECHANISM OF WATER TRANSFER IN CATALYSTS AND ADSORBENTS

N.A. Yazykov, A.D. Simonov, V.N. Parmon

J. Molec. Catal. A: Chemical, 158 (2000) pp. 467-470.

Drying is a key stage in numerous technological processes in the preparation of adsorbents and catalysts. A very efficient method preserving the quality of dried material is adsorption-contact drying. To calculate the rate of the mass transfer in the process of the adsorption-contact drying, it is necessary to have the data on the ratio between the gas-phase and liquid-phase transfer of moisture. A method to determine the rates for gas-phase and liquid-phase transfer of moisture in the process of mass transfer in porous materials is suggested. The data obtained agree well with the existing theoretical concepts about the liquid-phase transfer of moisture under the mechanical contact of two porous bodies.

OLEFINS FORMATION BY OXIDATIVE DEHYDROGENATION OF PROPANE OVER MONOLITHS AT SHORT CONTACT TIMES

V.A. Sadykov, S.N. Pavlova, N.F. Saputina,
I.A. Zolotarskii, N.A. Pakhomov, A.N. Salanov

Stud. Surf. Sci. & Catal.,
Proceedings of the 12th International Congress on Catalysis,
130B (2000) pp. 1907-1912.

A specially designed tubular microreactor allowing to rapidly quench reaction products was used to test performance of Pt supported onto corundum micromonoliths in the reaction of propane oxidative dehydrogenation at short contact times. Promoters known as dehydrogenation catalysts (tin, zinc aluminate spinel, transition metal pyrophosphates) were used and reaction mixture composition was tuned to increase propylene yield. FTIRS data on propane interaction with a model Pt/SiO_2 system helped to analyze the possible routes and limits of propylene yield improvement

PROPAGATION OF THERMAL WAVES IN A CATALYST BED DURING THE OXIDATION OF SULFUR DIOXIDE

A.P. Gerasev

Russ. J. Phys. Chem., 74 (2000) pp. 1077-1082.

A thermodynamic model for a quasi-homogeneous oxidation of sulfur dioxide in a stationary catalyst bed was developed. It was demonstrated that there is a one-parameter set of autowave (limited) solutions to the mathematical model for the propagation of thermal waves. An analysis of the distribution of the local production of entropy over the space–time coordinate was performed. The total production of entropy in a distributed open system was shown to be a function of the autowave solution. A single solution satisfying the principle of minimum production of entropy (lowest energy dissipation) was selected from the continuum of auto-wave solutions. A variational formulation of the procedure for calculating the characteristics of thermal waves was suggested, which is more advantageous from the practical point of view than the procedure of truncation (setting at zero) of the chemical reaction rate.

NONEQUILIBRIUM THERMODYNAMICS OF HEAT WAVES IN A CATALYTIC BED. FUNCTIONAL OF AN AUTOWAVE SOLUTION

A.P. Gerasev

Combustion, Explosion & Shock Waves, 36 (2000) pp. 329-336.

The paper deals with thermodynamic description and construction of nonequilibrium entropy of a fixed catalyst bed in approximation of simplest (quasihomogeneous) model during a reversible reaction. The physical nature of slow heat waves is shown to obey the second law of thermodynamics, and the total production of entropy in a distributed open strongly nonequilibrium system is the functional of an autowave solution of the mathematical model. From the one-parameter set of autowave solutions, the functional minimum corresponds to the unique physical meaningful solution. The variational problem is formulated using the principle of entropy production minimum in the heat wave. Methods of nonequilibrium thermodynamics are used for justification of the procedure of 'cutting-off' the reaction rate.

THE TECHNIQUE OF MICROPORE SIZE DISTRIBUTION RECONSTRUCTION ON THE BASIS OF THE DUBININ THEORY OF VOLUME FILLING

G.Yu. Cherkashinin, M.K. Ismakaev,
A.V. Bubnov, V.A. Drozdov

Inverse Problems, 16 (2000) pp. 1421-1440.

A simple numerical algorithm for the reconstruction of micropore size distribution (MPSD) dealing with equilibrium adsorption isotherm data is presented. The mathematical model is based on the theory of volume filling of micropores (TVFMP) and the regularization method was used in the numerical algorithm for solving the TVFMP inverse problem. The two different approaches to inversion of the initial integral equation, namely, the MPSD reconstruction in terms of both micropore volume and micropore surface area, are analyzed. The various exponent values in the local Dubinin-Astakhov isotherm and two types of smoothing functionals are analyzed with the aim of studying their influence on the results of the MPSD reconstruction. On the basis of numerical experiments with the various model distributions, a simple scheme choosing the regularization's optimal parameter is proposed. This scheme allows one to use observed data in calculations, obtained during only one experimental run, that essentially decrease the time of a cycle; for example an adsorption experiment – a MPSD reconstruction. The N_2 adsorption isotherm for the properly characterized molecular sieve, carbon HGS-638, was used for testing the proposed technique. The results of MPSD reconstruction calculated in terms of the surface area model are in good agreement with the known data for this sample. The present technique can be applied to analysis of a wide class of micropore materials, such as zeolites, molecular sieves and carbon sorbents.

SCIENTIFIC PUBLICATIONS

JOURNAL PUBLICATIONS AND MONOGRAPHS

1. **E.M. Al'kaeva, T.V. Andrushkevich, G.A. Zenkovets, G.N. Kryukova, S.V. Tsybulya**,
   Formation of Active State in Vanadium-Titanium Oxide System Regarding to Reaction of Oxidation of β-Picoline to Nicotinic Acid,
   Catal. Today, 61(1-4) (2000) pp. 249-254.
2. **M.P. Anisimov, (P.K. Hopke, S.D. Shandakov, I.I. Shvets)**,
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