

Institute of Physical Chemistry "I.G.Murgulescu" of the Romanian Academy

<http://www.icf.ro/>Contact: Director Prof. dr. Mihai Popa, mpopa@icf.ro

Address: 202 Splaiul Independentei St., P.O.Box 194, 060021 Bucharest - 12, Romania, Tel: +40.21.224.88.95, Fax:+40.21.312.11.47

Oxide Materials Science Laboratory

The activity of the **Oxide Materials Science Laboratory** is developed in the frame of the "Physical Chemistry of Oxide Materials" Program. The program is divided in three projects:

1. **"Phase equilibria and reaction mechanism in oxide systems"**, devoted to scientific foundations for designating and developing classical and non-conventional methods for obtaining new oxide materials and to characterize these materials from structural and technological point of view. The studies are oriented in the field of SnO₂-based semiconductors, Bi₂O₃-based superconductors and ionic conductors, Nb₂O₃-based dielectrics and hexagonal ferrites. The phase equilibria studies are approached by experimental and calculation methods.

2. **"Correlation between structure and properties of vitreous systems"**, devoted to studies concerning the correlation between composition-structure-thermal history of glasses containing PbO and ZrO₂ and their properties. The chemical and thermal properties of the glasses are mainly under evaluation. Such vitreous systems are of interest for waste inertization, optical application and coatings. Special attention is given to IR spectroscopic structural determination of the vitreous state, while the crystallization tendency is evaluated by DTA measurements. The chemical stability of the glasses is determined by leaching and chemical analysis of the dissolved ions.

3. **"Oxide systems obtained by sol-gel method"**, devoted to study of the sol-gel chemistry in systems leading to oxide and hybrid materials as well as to obtaining of films, powders and nanocomposites.

- In the sol-gel film preparation the most important work was oriented to obtaining of nanostructured monocomponent TiO₂, SiO₂, SnO₂, Al₂O₃, Fe₂O₃, HfO₂ and binary ITO, LiCoO₂ SiO₂-MO (where M=Cu, Co, Fe) TiO₂-MO (where M=Cu, Co, Fe, V), based films with several, specific applications, as: waveguides, sensors, catalysts, anticorrosive protection.

- By sol-gel method, nano-sized powders were also obtained in monocomponent Al₂O₃, TiO₂, SiO₂, MgO, Fe₂O₃, CeO₂, ZrO₂ systems as well as in binary and poly-component ones. The powders were used to obtain advanced ceramics of tialite, mullite, spinel type or were used as catalysts and as anticorrosive inhibitors.

- In the field of sol-gel nanocomposites studies were directed to preparation and characterization of the sol-gel oxide and hybrid nanocomposites of different types in SiO₂ - based systems and in

Head of the Laboratory: Dr. Maria Zaharescu, senior researcher, mzaharescu@icf.ro

Chemical Thermodynamics Laboratory**Research Activities**

1. **Thermodynamics of the gaseous and condensed systems in the pure phases and at the equilibrium between phases.**

1.1. **High-Temperature (700-1200°C) Phase Transformations. Solid State Thermodynamics.**

- Thermodynamics of the condensed systems in the pure phases and at the equilibrium between phases.

- The thermodynamic study of some oxide systems and new inorganic materials with special electric and magnetic properties.

- The thermodynamic characterisation of micro and nanostructured materials with different applications (catalysis, semiconductors, the energy storage and production, CMR compounds).

- The investigation of the thermodynamic properties of nonstoichiometric oxides (e.g. transition or other metal oxides) with special electric and magnetic properties.

- Solid electrolytes; Electrochemical sensors; Solid oxide fuel cells

Contact person: **Dr. Speranta Tanasescu, stanasescu@icf.ro**

1.2. **The Vapour - Liquid Equilibria (VLE) Measurements**

- Vapour-liquid equilibria (VLE) measurements for organic mixtures at low and normal pressure; application to separation processes

- Gas solubility measurements in high boiling point liquids or solid powders; application to supercritical fluid technology

- Vapour-liquid equilibria measurements in systems with chemical reaction; application to reactive separation processes

- Thermophysical properties measurements for pure liquids and mixtures at atmospheric pressure

- Thermodynamic modelling and processing of experimental thermodynamic data

Contact persons: **Dr. Alexandru Barhala, abarhala@icf.ro**

Dr. Mariana Teodorescu, mateodorescu@icf.ro

Head of the Laboratory: Dr. Speranta Tanasescu, senior researcher stanasescu@icf.ro

binary SiO₂-TiO₂ and SiO₂-ZrO₂ systems. Several oxides (Fe₂O₃), dyes (rodamine, methyl red, purple of brom cresol) and enzymes (glucose oxidase, protease, serine) were experienced as active phases in the obtained nanocomposites.

Between 2000-2004 the Laboratory contributed in 150 scientific papers. A number of 101 papers were published in referred journals (66 in foreign journals and 35 in Romanian ones) and 51 papers were published in the Proceedings of international (34) and national (15) conferences.

Two chapters of the "Micro and Nanostructures", Serie 2 and on chapter of the same publication, Serie 3, edited by the Ed.Academiei Romane, Bucharest, were realized by researcher working in the Oxide Materials Science Laboratory.

In the discussed period the Laboratory was involved in 2 projects granted by the Romanian Academy, as coordinator and contributed in other 28 National Projects, as following: 3 projects granted by the CNCSIS, 11 projects in the frame of MATNANTECH National program, one project granted by the CERES National Programme, 1 BIOTECH project and 12 Research of Excellency National Projects (CEEX).

The Laboratory is also highly involved in international research cooperation. For the time being it collaborate in 6 *inter-academic collaboration with France, Czech Republic, Bulgaria, Serbia and Hungary*, in a thematic network "Polar electroceramics" in the frame of the FP5 Program, two COST Actions, 525 "Grain Boundary Engineering" and COST Action 539, *Electroceramics from Nanopowders Produced by Innovative Methods (ELENA)*, a NATO Collaborative Linkage Grant "Microwave and corrosion behaviour of Ceramer-conductive polymer composite coatings" and n IP FP6, Priority 3-NMP project. Advanced environmentally friendly multifunctional corrosion protection by Nanotechnology". In the same time the *Head of the Laboratory is the President for the 2005-2006 period of the South-East European Consortium on Nano-Science and Technologies: Nanostructured Materials and Devices (COSENT)*.

The laboratory possesses the infrastructure for preparing oxide materials by sol-gel, at room and high temperatures and in normal or controlled atmosphere. Methods of thermal and structural characterization are also available, as: DTA/TGA and DSC equipment (Mettler-Toledo), FTIR spectrometer (Nicolet), programmed furnaces up to 1250°C (Lynn and Norbertham).

1.3. Thermochemical characterization of the biological interest compounds

- Thermochemical characterization of the biological interest compounds (amino-acids, collagen etc)

- Thermodynamics of binding interactions in water-cyclodextrin system

Contact person: **Dr. Iulia Contineanu, iconti@icf.ro**

International Projects and Scientific Collaborations

- Participant in EU project on "Improving the understanding of the impact of nanoparticles on human health and the environment", ImPart CA, Programme: Priority 3 - NMP, 2005-2007

- Participant (2004 - 2005) in EU COST Action 525: Advanced Electroceramics: Grain Boundary Engineering, Project "Structural and dielectric studies of incipient ferroelectrics"

- Participant in the COSENT - South-East European Consortium on NANO - Science and Technologies: Nanostructured Materials and Devices as member, beginning with 2004 Romania

- Bulgaria bilateral academic cooperation, "Optimization of Hydrogen and Oxygen Electrodes for Proton Exchange Membrane Fuel Cell's Application" JRC Project, beginning with January 2005

- The scientific cooperation with the Institute of Metallurgy and Materials Science "Aleksander Krupkowski", Polish Academy of Sciences. Agreement on the scientific collaboration 2002-2004 and JRC Project 2003-2004.

- The scientific cooperation with ETH Zürich, Department of Materials
- Institute of Nonmetallic Materials, Thermodynamic Group, Switzerland concerning "The thermochemical properties of the compounds in the La-Sr-Mn-O system". Agreement on the scientific collaboration 2001-2003.