SOLID-STATE CHEMISTRY

Review and development of teaching materials and definition of terms

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INTRODUCTION

Solid-state chemistry appeared in the second half of the 20th century as a new branch of modern chemistry related to the **development of high technological materials**. Essential parts of solid-state chemistry are as follows:

- Models
- Theoretical approaches
- Experimental techniques and data

Industry has to solve many problems in the application of materials from microelectronics, communication, information, energy conversion and storage, construction, electronic packaging, domestic and advanced ceramics, to mineral technology such as rare earth compounds, borophosphates, zeolites as molecular sieves, or borophosphosilicates as packaging materials.

Inorganic chemistry has become a very important field of chemistry because most high technological materials have an inorganic origin. Some minerals that are found in nature possess conducting (sulfides), piezoelectric (perovskites), magnetic (ferrites), or ion exchange (zeolites) properties.

Inclusion of solid state-chemistry topics in inorganic chemistry textbooks was inevitably found to be extremely important for emerging new technologies.

Our aim is to educate students at the **undergraduate** and **graduate** level about solid-state chemistry, because this topic was not included in the curricula chemistry departments as a required course in most countries.

On the other hand, the significance of solid-state chemistry in advanced materials in recent years has led to a large increase number of MS and PhD materials science students in many universities and, in turn in, modern research laboratories.

The following specific projects were developed by the **INORGANIC CHEMISTRY DIVISION - COMMISSION HIGH TEMPERATURE MATERIALS AND SOLID STATE CHEMISTRY** and the **COMMITTEE ON TEACHING OF CHEMISTRY**:

- **COLLECTING, TESTING, AND DISSEMINATING EXPERIMENTS IN SOLID-STATE AND MATERIALS CHEMISTRY**

> to provide wider training to undergraduate and graduate students not only in the fields of theoretical and experimental solid state and materials chemistry, but also to provide additional background to physical, analytical, organic, biochemistry or polymer chemistry students.

- **DEFINITION OF TERMS FOR DIFFUSION IN THE SOLID STATE**

> IUPAC Recommendations describing the migration of host and foreign species through solid materials

MAIN DIRECTIONS IN THE PROGRESS OF SOLID-STATE CHEMISTRY

1. Preparation of materials

   Cement, ceramics, glasses, polymers, composites, electronic materials with certain characteristic properties such as ferrites, lasers, TV phosphors, light-emitting diodes, production of one dimensional conductive structures, shift structures causing nonstoichiometry, new ceramic materials with unusual functional properties, and, finally, synthesis of semiconductors and superconductors

2. Reactivity of solids

   Role of defects in the mechanism of the solid-state reactions

3. Mass transfer processes in a solid state

   - Laws determining mass transfer processes when diffusion in solids is accompanied by a chemical reaction
   - Synthesis and properties of fast ion conductors, development of sensor devices based on ion conductivity solid-state eletrochemical cells

4. Solid-state reactions under extreme conditions

   Initiation of the processes by electricity, magnetic field, electromagnetic radiation, or mechanical impulse

EXAMPLES OF HIGH TECHNOLOGICAL MATERIALS

Ferrites: (Cd, Mg, Mn) Fe_2O_4 used in computer memories

Lasers: ruby, YAG (yttrium-aluminium-garnet), $Na_3Nd(P0_4)_2$

Thermistors: mixed oxides that can be used as detectors

Light-emitting diodes: (LED) GaAsP (numeric readout on calculators)

Optical Fibers: for communication and data transmission

Semiconductors: Si or Ge doped with P or B or compound semiconductors such as $CuFeS_2$

Piezoelectric materials: as sound detectors or sensors in electronic balances ($BaTiO_3$)

Nitride ceramics: Si_3N_4 replaces metals in gas turbines and automobile engines

Bioceramics: tetracalcium phosphate ($Ca_4P_2O_9$), apatite ($Ca_5(PO_4)_3OH$)

Superconductors: yttrium barium copper oxide ($YBa_2Cu_3O_{7-x}$)

Composites: polymers + ceramics + metals or other matrices with reinforcing fillers

Carbides: boron carbide (BC), silicon carbides (SiC)

COLLECTING, TESTING, AND DISSEMINATING EXPERIMENTS IN SOLID-STATE AND MATERIALS CHEMISTRY

The experiments will be classified by categories, based on the intended users:

- In junior undergraduate laboratories (1st and 2nd year)
- In senior undergraduate laboratories (3rd and 4th year)
- Laboratory for the 4th year elective courses, such as Solid-State Chemistry and Inorganic Materials or Structural Inorganic Chemistry
- Advanced experiments for senior undergraduate students as projects or for Master’s students as a laboratory course

Individual experiments can be selected, and changes can be made, according conditions and reactants, that will widen the scope of the project.

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TOPICS OF THE EXPERIMENTS

- Synthesis of polycrystalline or single crystal materials by solid-solid, solid-gas, chemical vapor deposition (CVD) to produce thin films or surfaces, solution hydrothermal, sol gel, microwave, etc., methods
- Characterization using different instrumental and chemical techniques such as XRD, IR , DSC, DTA, SEM, NMR, AAS, ICP, etc.
- Determination of magnetic, electrical, piezoelectric, optical, thermal, and mechanical properties

Two sets of laboratory experiments are being reviewed. Some experiments have been tested and were found to be feasible and applicable. Some of them can be useful only in a well-equipped solid-state laboratory.

First set:

- Preparation and characterization of barium titanate (BTO) and BTO 'posistors'
- Synthesis of ferroelectric $BaTiO_3$ via sol-gel route
- Fabrication of thin film CdSe photoelectrochemical solar cell and measurement of its efficiency
- Synthesis and study of the high-T_c superconductor $YBa_2Cu_3O_{7-\delta}$.
- Synthesis of a '123'-superconductor
- Ionic conductivity in glass
- Synthesis of luminescent materials
- Synthesis of ferrimagnetic $BaFe_{12}O_{19}$
- Synthesis of X-zeolite

Second Set:

- Synthesis and properties of $LaCoO_3$ and
- $La_{0.6}Sr_{0.4}CoO_3$
- Preparation and characterization of an intermetallic compound, V_3Si
- Synthesis and crystal growth of MoO_2 and characterization
- Synthesis and magnetic characterization of a hard magnetic material, $BaFe_{12}O_{19}$
- Synthesis and intercalation studies on the layered transition metal dichalcogenides, 2H-TaS_2 and 2H-$MoSe_2$
- Synthesis and characterization of a metal-cluster compound, $Cu_2Mo_6S_8$

Additional experiments include the following:

- Synthesis and characterization of lanthanide phosphates
- Synthesis of characterization of tetracalcium phosphate, $Ca_4P_2O_9$, a dental cement
- Preparation of gadolinium tetraphosphate, $Gd_2P_4O_{13}$, and a study of its structure by XRD and IR methods
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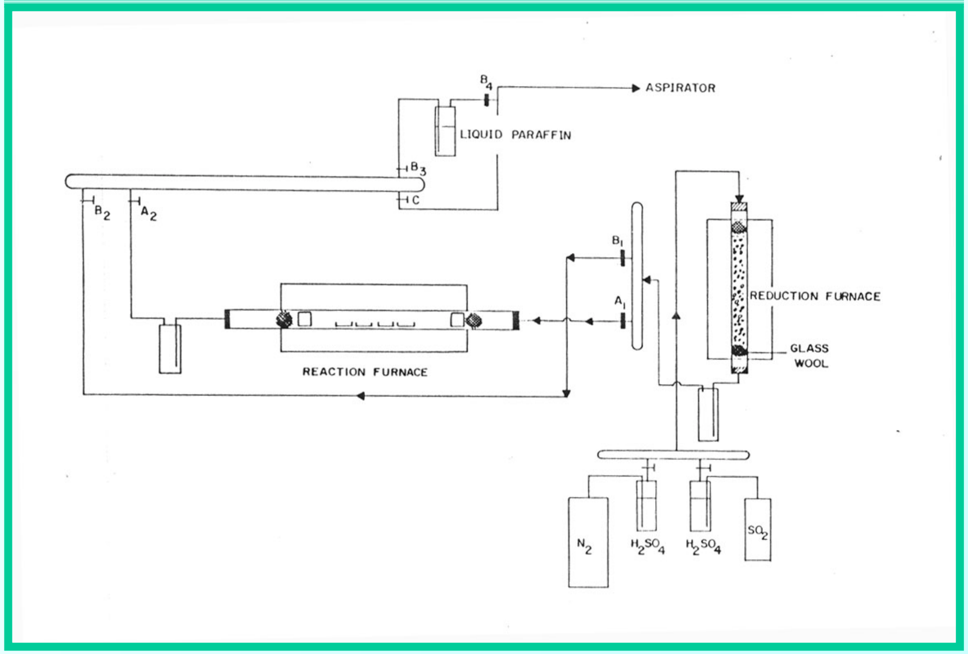
- Preparation of copper iron sulfides by solid-gas reactions
- Synthesis, characterization, and conducting properties of $YBa_2Cu_3S_{6-x}$
- Synthesis of sodium dichromate, $Na_2Cr_2O_7$, and sodium chromate, Na_2CrO_4,
- Preparation of $YBa_2Cu_3O_{7-x}$ by using citrate synthesis

Example of presented experimental setup



Experimental setup for the synthesis of $YBa_2Cu_3O_{7-x}$

TERMINOLOGY FOR DIFFUSION IN THE SOLID STATE

IUPAC Recommendations - *Pure Appl. Chem*. Vol. 71 , No. 7, pp. 1307–1325, 1999; by M. Kizilyalli, J. Corish, and R. Metselaar.

This document provides **definitions of terms and processes** that are used in describing the migration of host and foreign species through solid materials. Both the phenomenological theory of diffusion and the detailed atomistic mechanisms by which atom transport occurs are treated. Also included are the various types of gradients such as electrical, chemical, thermal, and mechanical, which provide the driving forces for diffusion.

The definitions in this document relate specifically to the solid state and are intended for the professional scientist, but they will not necessarily meet all the needs of the specialist chemist, physicist, or material scientist. A system of cross-referencing has been used in which italicized terms are known by more than one name.The references cited in the bibliography are not unique but provide additional reading on specific definitions.