

# Solids: Dynamics and Kinetics in Siegen

By Hermann Schmalzried \*

German physical chemists are organized in the "Deutsche Bunsengesellschaft". Their annual meetings on varying topics of current interest and importance are held each year at a different university, this year's, the 88th, being held from May 4.-6. in Siegen. The physical chemistry of solids links the two basic solid state sciences, chemistry and physics. The dramatic increase in effort and progress in the solid state sciences has been triggered by the growing need of materials in our technical civilization. As a response, this year's main topic of the "Bunsen-meeting" was formulated as "Solids: Dynamics and Kinetics".

Solid state kinetics deal with chemical processes in solids and particularly with their behavior within time. These processes occur under the influence of thermodynamic driving forces which act on the atomic particle ensembles of the solid. An example is the widely studied oxidation of metals in a tarnishing process.

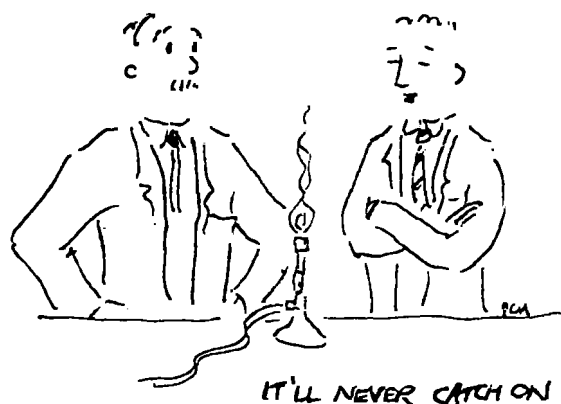
Solid state dynamics deals with the restricted, and often correlated motions of localized atomic particles, an example of which is the vibration of an atom or a group of atoms in a crystal. Traditionally, kinetics is more the domain of the chemist, whereas dynamics has rather been investigated by the physicist.

The key problem in the physical chemistry of solids is the explanation of the parameters of phenomenological kinetic theory in terms of solid state dynamics. In line with this theme, the three plenary lectures of the Bunsen-meeting started with a contribution by *H. Stiller* (Jülich/Berlin, FRG), discussing in detail individual and collective local particle motions in crystalline solids. *J. W. Cahn* (Washington, USA), whose theme was the physical chemistry of stressed solids, pointed out the fundamental differences between solids and fluids when it comes to the formulation of driving forces for solid state reactions: Solids can store elastic energies stemming from nonhomogeneous stresses. *G. Petzow* (Stuttgart, FRG) illustrated how to produce new materials with desired (mechanical) properties which are based on kinetic processes, through structure design; his examples were essentially taken from the field of nonmetallic inorganic compounds.

In addition to these plenary lectures, five more invited speakers gave progress reports on various topics of solid state research: *S. Clough* (Nottingham, UK) dealt with

"Gauge theory and molecular rotation in crystals",<sup>[1]</sup> *K. Funke's* (Münster, FRG) topic was "Transport and relaxation in ionic crystals", and *J. Rouxel* (Nantes, France) discussed "Reactivity and phase transitions in the chemistry of low dimensional compounds". The current state of solid state electrochemistry was reviewed by *A. R. West* (Aberdeen, UK) in his report on "Solid electrolytes", and the final contribution of *H. Sixl* (Frankfurt, FRG) dealt with "Organic solids: possible applications in optics and electronics".<sup>[2]</sup>

More than twenty oral presentations in three sessions and forty poster contributions from different research groups and various research fields clearly illustrated the breadth of solid state research and the interdisciplinary character of solid state physical chemistry. Physicists, chemists, polymer scientists, ceramists, and metallurgists all demonstrated the impact that basic research can have in helping to solve practical problems in material science.



Physical chemistry is, to a large extent, an experimental science. It is therefore interesting to review the main experimental methods applied in current research, as reflected in this meeting. One notes that solid state electrochemistry in its broad sense, and its classical experiments, still plays an important role, particularly when it comes to interfaces. Structure and dynamics are largely explored using neutron techniques, because their advantage of energy discrimination overrides in importance the general availability of X-rays. Solid state NMR, Mössbauer-effect, PAC-experiments and related experimental methods that probe the charge or spin density of the atomic surroundings are indispensable if one studies motion and transport on an atomic and a macroscopic

[\*] Prof. Dr. H. Schmalzried  
Institut für Physikalische Chemie und Elektrochemie  
der Universität Hannover, Callinstrasse 3-3A  
D-3000 Hannover 1 (FRG)

scale, although the more classical methods of sensing electromagnetic interactions between radiation and matter are being used continuously. In kinetic research it is found that in situ experiments, which for solids often mean high temperature experiments, are absolutely necessary. However, this makes the application of IR and visible light spectroscopy a most difficult task.

In a way it was interesting to note that electron microscopy is not used more by solid state physical chemists – at least in Germany. After all it is the (periodic) structure that distinguishes the solid from the fluid state and determines most of its properties including the kinetic and the dynamic ones, and high resolution electron microscopy offers spatial resolution on an atomic scale. Therefore it seems clear that electron microscopy will increasingly help us to understand the basis of solid state kinetics: the defect in the solid state.

Additionally, modern chemical analysis results in a much better characterization of the solids under investigation than ever before. This is most important with regard to the fact that it is always the crystal defect, including chemical impurities, that (as is well known in semiconductor technology) govern many of the crystal properties.

In conclusion: The Bunsen-meeting has again illustrated the interdisciplinary character of physical chemistry and has fulfilled its role of promoting the exchange of ideas, this year in particular between the different groups which work in the broad field of solid state science.

- [1] S. Clough, *Adv. Mater.* 1989, 296; *Angew. Chem. Int. Ed. Engl. Adv. Mater.* 28 (1989) 1124; *Angew. Chem. Adv. Mater.* 101 (1989) 1150.  
[2] H. Sixl, W. Groh, D. Lupo, *Adv. Mater.* 1989, No. 11; *Angew. Chem. Int. Ed. Engl. Adv. Mater.* 28 (1989) No. 11; *Angew. Chem. Adv. Mater.* 101 (1989) No. 11.

## Sol-Gel Processing in Bad Honnef

By Hans Reuter \*

The 52nd seminar of the Dr. Wilhelm Hereaus and Else Hereaus Foundation entitled "Sol-Gel Processing for Glasses, Ceramics and Inorganic-Organic Polymers" was held from Monday, May 22nd, through Wednesday, May 24th, 1989 at the Physikzentrum in Bad Honnef, FRG.

Basically the expression "Sol-Gel Process" means the formation of an amorphous solid, the gel, starting from a homogeneous liquid, a molecular dispersion or colloidal solution. The great amount of scientific and technological interest devoted to this process ranges from molecular chemistry to material science. One aim of the seminar was to bring together, in a small circle, scientists from these different fields to discuss in an interdisciplinary manner the numerous aspects of sol-gel-processing. Twenty invited speakers and about thirty further participants attended the meeting coming from both university laboratories and industry.

An instructive overview of the present industrial application of the sol-gel technique was given in the paper "Sol-Gel 1969–1989, Paths of Development and Products, Especially the Newer Ones" from H. Dislich (FRG), who also showed some remarkable examples of industrially fabricated, sol-gel derived products. Complementing this, D. R. Uhlmann (USA) illustrated in his lecture "General View of Sol-Gel

Technologies" not only the present state of the art developments and the numerous unsolved problems but also the future possibilities of the technology.

One main problem is, that there is only little known about the chemistry which happens during the sol to gel transformation. This was analyzed in two papers. In the first one, "Monoorgano Tin Compounds as Model Substances for the Investigation of the Sol-Gel Process", M. Jansen (FRG) showed that with organometallic precursors it is possible to isolate crystalline oligomers, which can be studied by X-ray structure analysis in order to see directly how i.e. the solvent may influence the reaction path. In the second paper "Sol-Gel Chemistry of Transition Metal Oxides", C. Sanchez (France) demonstrated, using titanium alkoxides as an example, not only the role of solvent molecules but also that of other chemical additives like catalysts, stabilizing agents or drying control chemical additives.

The processes following gel formation, like drying and densification, were reviewed in the lectures of G. W. Scherer (USA) who talked about "Hypercritical Drying", "Aging and Syneresis" and "Sintering of Gels", while D. J. Brinker (USA) discussed the "Fundamentals of Thin Film Formation from Sol-Gel Solution" and the "Spinnability of Silica Sols: Structural and Rheological Criteria" dealing with the more practical aspects.

New experimental paths were pointed out by C. Rüssel (FRG) "Non-Oxide Ceramics by Sol-Gel Techniques" mak-

[\*] Dr. H. Reuter  
Institut für Anorganische Chemie  
Universität Bonn, Gerhard-Domagk-Strasse 1  
D-5300 Bonn 1 (FRG)