Gabriele Leoff

Schott Glas
Mainz, Germany

Milestones for Glass Science

This year's Otto Schott Research Award was granted to Professor Dr. Reinhard Conradt (Institute of Mineral Engineering, Chair of Glass and Ceramic Composites, RWTH Aachen) and to the Russian team, Dr. Boris Anatoljevich Shakhmatkin and Dr. Natalia Mikhailovna Vedishcheva (Institute of Silicate Chemistry, Russian Academy of Sciences, St. Petersburg) for exceptional scientific achievements.

In annual alternation with the Carl Zeiss Research Award, Schott seeks to inform a broader public of new scientific achievements in the fields of glass and glass ceramics or optics while also promoting the significance of glass science for technical progress. The quality of the work reflects the top level of glass science internationally.

Prof. Conradt received the award "for his conception of a highly versatile approach to thermodynamic modeling of oxide melts and glasses based on constitutional relations of equilibrium phases and for the pioneering results achieved by this approach in the evaluation of physical and chemical properties, particularly chemical resistance, of technical multi-component glasses."

Dr. Boris Anatoljevich Shakhmatkin and Dr. Natalia Mikhailovna Vedishcheva, received the award "for the development of a rigorous thermodynamic model of oxide melts and glasses based on compound equilibria and for the impressive results obtained by applying this model to the evaluation of physical properties of two-component glass forming systems."

The award, with a total prize money of 25,000 euro was presented on July 1st, 2001 during an international congress on glass science in Edinburgh (Scotland) ■

Precise and Practical

Prof. Dr. Gerd Mueller, Director of the Fraunhofer Institute for Silicate Research in Wuerzburg and member of the Otto Schott Research Award Committee addresses the usefulness of the research.

Has the reliability of these models been tested?

Over the last decade an impressive and, in the opinion of the Award Committee, convincing amount of evidence has been presented by both groups that the models work and yield reliable results – in many instances with the same degree of accuracy as the experimental data.

This is true not only for properties that are directly related to thermodynamic functions and their derivatives such as volume, thermal expansion or heat capacity, but also for transport properties like viscosity, diffusion or ionic conductivity.

Do you expect the models to be of practical use in the near future?

The Otto Schott Award Committee is of the opinion that the thermodynamic models will be of great merit also for very practical purposes. Schott Glas therefore actively encourages close cooperation between the award winning groups.

What does that mean in concrete terms?

Hopefully software packages will become available soon which can be used as tools for the development and optimization of technical, multi-component glasses. The models today calculate properties from compositions. With the power of informatics and computers it can be expected that the inverse problem, namely suggesting suitable compositions for desired sets of properties, will also be solved readily ■

— INTERVIEW —

From Structure Analysis to Glass Technology

Prof. Dr. Reinhard Conradt

The award ceremony took place during this year's international glass congress held by the International Glass Commission on Glass in Edinburgh, Scotland. From left to right: Curator Prof. Dr. Gerd Mueller, Dr. Boris Anatoljevich Shakhmatkin, Dr. Natalia Mikhailovna Vedishcheva, Prof. Reinhard Conradt and Schott Board Member Dr. Udo Ungeheuer.

What is the relationship in principle between the chemical composition of a glass and its properties? This is a question that has exercised the minds of scientists and technologists since the beginnings of systematic glass research in the 19th century. Otto Schott recognized at an early stage the need to approach the question on the basis of a very broadly structured scientific concept:

"A systematic study of the phenomena of glass melting comprising its whole inorganic nature has not yet been attempted; we lack, therefore, much in this area before we will be in a position to determine the reactions with certainty on the basis of fixed laws as is the case with aqueous solvents at normal temperature."

Otto Schott, 1880, quoted by W. Vogel, Glaschemie (Springer Verlag, Berlin 1992)

The nature of glass, its transparency, its homogeneity and its isotropy, suggest simplicity – yet the opposite is the case. With metallic materials, the issue has been largely settled. However glass, as a "special state of matter," has eluded a more fundamental quantification again and again. In deducing the properties of glass from its composition, one has to collect experimental data, link it, evaluate it statistically and then interpolate or extrapolate into unknown territory.

Thermodynamics: a New Method

In recent years a new, fundamental strategy has emerged. Attempts to understand the properties of a glass largely on the basis of its structure have been abandoned. This route is one which, in spite of enormous research efforts, has thus far only resulted in explanatory, qualitative evidence. Instead thermodynamic methods have been enlisted and applied systematically to the situations encountered in multi-component glasses. The method is, of course, not as transparent as a structural interpretation, but it does supply quantitative evidence. The glass is described via its energy difference to a crystalline object (or reference system) with the same chemical composition.

Complex Sequences can be Analyzed

Tracking this reference system is simple for mono-component glasses (e.g. fused silica and cristobalite); it can also be done for glasses with many components using geochemical methods. In principle this has finally opened up the use of comprehensive thermodynamic databases and books of tables for glass technology. Now it is possible to computer-model quite a few of the properties of glass, such as chemical resistance, before carrying out the first trial melt and the first corrosion test. With further development of the process it can be expected that it will be possible to significantly reduce the amount of work based on trial and error, thus saving time and costs.

The new modeling strategy is, however, not limited to just forecasting the properties of glass. Complex reaction sequences, in which a glass or its melt is involved as part of the reaction, can now be subjected to quantitative treatment. Technologically relevant examples are the determination of the energy required for the fusion of glass batches or the evaporation of individual components in a melt resulting from the effect of a furnace atmosphere ■

Model Supplies Reliable Results

Dr. Boris A. Shakhmatkin
Dr. Natalia M. Vedishcheva
Institute of Silicate Chemistry of the Russian Academy of Sciences
St. Petersburg, Russia

Glass is one of the oldest man-made materials, already known in 3000 B.C. to the ancient Egyptians. Over the millennia, man has experimented with glass to achieve different properties and effects. Today a broad palette of glass art, consumer glassware and industrial glasses is available, as well as a number of methods and processes for the analysis and modification of the physical and chemical properties of glasses.

Attractive Alternatives

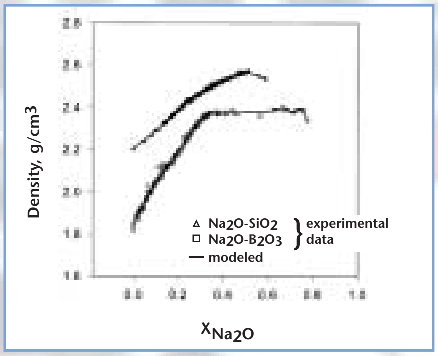
Researchers today have an extensive amount of experimental data on the properties of oxide glass-forming systems, upon which many of our industrial glasses are based. Sophisticated new techniques such as MAS-NMR, EPR and EXAFS enable a deeper insight into the glass structure. Traditionally changes in the structure were believed to cause changes in the glass properties. However, neither a better understanding of the structure/ property relationship in a given system nor detailed knowledge of its properties as such, can help to predict a priori how a system will react upon the introduction of new components. To answer this question, an entirely new study would have to be conducted, a time and labor intensive undertaking, especially when multi-component glasses are involved. Therefore the possibility of modeling the behavior of glass-forming systems is a very attractive alternative.

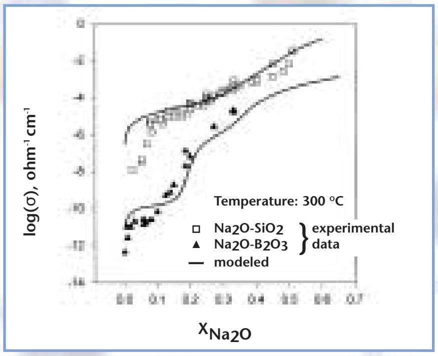
Thermodynamic modeling based on the model of associated solutions enables a large variety of properties of glasses to be predicted on a unified basis, over extremely wide concentration and temperature regions, without use of adjustable parameters and with a high degree of accuracy. The approach applies to systems formed from any number of components with different chemical natures (basic and acidic oxides). The formalism of the model of associated solutions enables the equilibrium concentrations of all the species (the salt-like products and the unreacted oxides) present in a glass to be determined as a function of glass composition, temperature and pressure. With this information the following properties of glass can be modeled: density, refractive index, heat capacity, electrical conductivity, diffusion coefficient of ions as well as the red-ox equilibria in glasses, their chemical durability and the ability to crystallize.

Successful Application

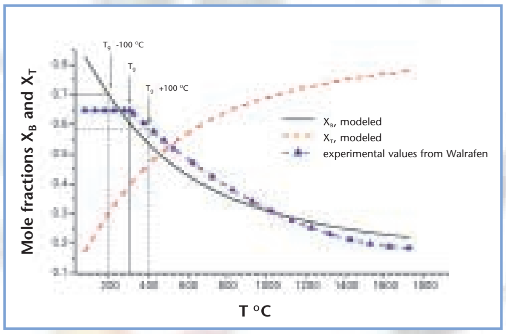
However in theory, the range of physical properties, which can be calculated using the model of associated solutions is actually considerably broader. Analytical expressions have been derived therefore for the isothermal compressibility, the coefficient of thermal expansion, the magnetic and mechanical properties of glasses.

In addition to glass properties, structural characteristics can also be modeled, for example the distribution of the basic structural units as a function of the glass composition and temperature. A good agreement between the model and experimental dependencies points to the fact that the thermodynamic approach can successfully be used for estimating the influence of temperature on the glass structure ■





Calculated dependencies for the density and electrical conductivity in sodium silicate and sodium borate glasses together with the corresponding experimental data (from O.V. Mazurin et al., Properties of Glasses and Glass-Forming Liquids, Nauka, Leningrad, 1975). The precision of the modeling corresponds to the precision of the experimental measurements.



Example of the temperature distribution from B_3O_6-boroxol rings (X_B) and BO_3-triangles (X_T) in glassy boroxide (T_g is the glass transition temperature. Experimental data based on results from G.E. Walrafen et al., J. Chem. Phys. 72 (1980), S. 113).