

**MS10.02.03 TOWARD A FULL PARTIAL STRUCTURE OF  $v\text{-GeO}_2$ .** M.-L. Saboungi, D.L. Price, Argonne National Lab, Argonne, Ill. 60439, and A.C. Barnes, University of Bristol, Department of Physics, Bristol, UK

The acquisition of partial structure information—the structural correlations between all pairs of elements—represents the ultimate goal in analysis of disordered systems. In favorable cases, full information is obtained from neutron diffraction (ND) with isotopic substitution, if suitable isotopes are available, in others from anomalous x-ray diffraction (AXD) if the absorption edges lie at suitable energies. In the least favorable case, one may resort to a combination of the two methods. We report an analysis of the structural data from such a case,  $v\text{-GeO}_2$ . The extracted partial structure factors are presented, with a discussion of present limitations of the method. A comparison with computer simulations will be presented.

This work was supported by the U.S. Department of Energy, Materials Sciences, Basic Energy Sciences, under Contract No. W-31-109-ENG-38

**MS10.02.04 DAFS STUDY OF INTERMEDIATE-RANGE ORDER IN  $v\text{-GeO}_2$  and  $v\text{-GeSe}_2$ .** D.L. Price, M-L Saboungi, Argonne National Laboratory, Argonne, Illinois 60439, P. Armand, University of Montpellier, Montpellier, France and D. Cox, Brookhaven National Laboratory, Upton, New York 11973

The Diffraction Anomalous Fine Structure (DAFS) technique combines the short-range selectivity of XAFS with the long-range structural analysis of x-ray diffraction, and provides structural information not available from these techniques alone or in combination. As such, it should throw light on the question of what local atomic arrangements are involved in the scattering that gives rise to the first sharp diffraction peak (FSDP). We have carried out DAFS measurements around the first two diffraction peaks in two typical glasses,  $\text{GeSe}_2$  and  $\text{GeO}_2$ . We discuss the origin of the FSDP and other information that may be drawn about intermediate-range order in the glasses, and prospects for the future use of the DAFS technique in disordered systems.

This work was supported by the U.S. Department of Energy, Materials Sciences, Basic Energy Sciences, under Contract No. W-31-109-ENG-38.

**MS10.02.05 EXPERIMENTAL Pt-Pt PARTIAL STRUCTURE FACTORS OF PLATINUM PYRIMIDINE GREENS BY AWAXS.** R. Serimaa, V. Eteläniemi, and M. Torkkeli, Department of Physics, P.O. Box 9, University of Helsinki FIN—00014, Finland; T. Laitalainen, J. Pitkänen, Department of Chemistry, P.O. Box 55, FIN—00014 University of Helsinki, Finland

The extraction of partial structure factors from anomalous x-ray scattering (AWAXS) data is an ill-conditioned problem, the statistical errors in the data seriously reducing the quality of the PSFs. An iterative way to apply the Tikhonov regularization method for solving partial structure factors (PSFs) from AWAXS data is presented [1].

The method is applied for solving the Pt—Pt PSF of platinum pyrimidine greens [2]. The materials, which are of interest due to their anticancer activity [3], contain several atomic species but only the absorption edges of Pt are accessible. Several Pt-greens [2], synthesized by varying ligand structures and reaction conditions, were studied by the AWAXS method. The results, which indicated that the major Pt-structures are mono- and dinuclear, are in contradiction with the widely accepted polymeric Pt-chain model. Studies of Pt-uridine green showed that the Pt-nuclearity can be varied by tuning the reaction conditions.

[1] R. Serimaa, V. Eteläniemi, O. Serimaa, A. Bienenstock and T. Laitalainen. *J. Appl. Cryst.* in press.

[2] T. Laitalainen, R. Serimaa, S. Vahvaselkä and A. Reunanen. *Inorg. Chim. Acta*, in press.

R. Serimaa, S. Vahvaselkä, T. Laitalainen and T. Paakkari. *J. Am. Chem. Soc.* 115 (1993) 10036.

[3] T. Okada, T. Shimura, H. Okuno. *Chem. Pharm. Bull.* 40 (1992) 264.

**MS10.02.06 THE STRUCTURE OF LIQUID METAL SURFACES: X-RAY REFLECTIVITY STUDIES†** P.S. Pershan<sup>1</sup>, M. J. Regan<sup>1</sup>, O. M. Magnussen<sup>2,3</sup>, B. M. Ocko<sup>2</sup>, M. Deutsch<sup>4</sup>, L. E. Berman<sup>5</sup>. <sup>1</sup>Division of Applied Sciences and Department of Physics, Harvard University, Cambridge, MA 02138, <sup>2</sup>Department of Physics, Brookhaven National Laboratory, Upton, NY 11973, <sup>3</sup>Current address, Abteilung Oberflächchemie und Katalyse University Ulm, Germany, <sup>4</sup>Department of Physics, Bar-Ilan University, Ramat-Gan 52100, Israel, <sup>5</sup>National Synchrotron Light Source, Brookhaven National Laboratory, Upton, NY 11973

The strong Coulombic and quantum interactions between the charged electron and ion fluids that constitute liquid metals were long predicted by theory and simulation to give rise to atomic layering at the free surface. This important prediction of atomic layering was verified recently by our group's x-ray reflectivity measurements on liquid gallium and mercury; however, unexpected differences between the surface layering for the two elements leave open fundamental questions that are reinforced by more recent results on the temperature dependence of the atomic layering of liquid gallium. Other experimental results will be reported on the oxidation of the liquid gallium surface, and self-assembled monolayers on mercury surfaces. Finally, discrepancies between the measured surface profiles and those from current theory and simulations will be discussed.

†This work has been supported by grants from the U.S. Department of Energy, DE-FG02-88-ER45379 and the National Science Foundation, DMR-94-00396 and DMR-95-23440. Brookhaven National Laboratory is supported by DOE Contract No. DE-ACO2-76CH00016. MD acknowledges support by the Bar-Ilan Research Authority.

**MS10.02.07 SAXS STUDIES OF POROUS GELS AND GLASS-NANOCRYSTALL MATERIALS.** A. F. Craievich, LNLS/CNPq, Campinas and IFUSP, Sao Paulo, Brasil

Introducing some degree of order in disordered systems may help to obtain interesting and useful materials. We will review recent synchrotron radiation small-angle scattering (SAXS) studies of materials having in common an initial amorphous structure and a final structure composed of nanocrystalline regions embedded in a disordered matrix.

The first investigation to be reported concerns a xerogel of  $\text{SnO}_2$  produced using the sol-gel route. The starting xerogel is a disordered and porous material. An X-ray diffraction study indicates the formation and slow growth of small crystallites (1). SAXS measurements during isothermal treatment demonstrated that the first stage of porosity evolution is governed by a coarsening mechanism, similar to that observed in biphasic alloys and glasses (2). Other investigated materials are silicate and borosilicate glasses in which semiconducting nanocrystals (CdS, CdSe, PbTe) nucleate and grow. The determination and control of the average size and the dispersion in size of the nanocrystals are necessary in order to tailor materials having prespecified properties. SAXS investigations helped to establish the heat-treatment procedure and composition choice which lead to materials composed of a glassy matrix containing spherical nanocrystals with radii in the range of 2–4 nm having a narrow size distribution (3). A third correlated research aimed at the obtention of a size-monodisperse system of semiconducting nanocrystals (CdS, CdSe) embedded in an amorphous and porous matrix. It involves the preparation of fine porous silicate sonogels using the sol-gel method assisted by ultrasound. The basic idea is that this matrix may induce heterogenous nucleation of semiconducting nanocrystals with a narrow size distribution. The characterization of this complex three-phase material, composed of an amorphous matrix, nanopores and nanocrystals, was performed by classical SAXS (4) and, more recently, using the anomalous SAXS technique (5).

#### References:

- 1-G.E.S. Brito et al., *J. Of Sol-Gel Sci. and Tech.* To be published (1996).
- 2-C.V. Santilli et al., *Phys. Rev. B*, 5, 8801 (1995).
- 3-A.F. Craievich et al., *Journl de Physique IV C8*, 3,376 (1993).
- 4-A.F. Craievich et al., *Nanostructured Materials*, 5,363 (1995).
- 5-D. Hummel et al., *J. Of Sol-Gel Sci. And Tech.* To be published (1996).