

**22.2-06** STRUCTURAL PROPERTIES OF  $ZnBr_2$  SOLUTIONS IN EtOAc. By G. Cubiotti, B. Ginatempo, G. Maisano and P. Migliardo, Istituti di Fisica and Fisica Teorica, Università, Messina, Italy.

X-ray diffraction patterns are presented for  $ZnBr_2$  solutions in ethyl-acetate, at different solute concentrations. It is observed that, even at low concentrations of  $ZnBr_2$ , the solute breaks the structure of the solvent, giving rise to diffraction patterns which put in evidence the strong Zn-Zn correlations. The diffraction data are correlated with existing EXAFS data in order to establish some distances between the constituents atoms. The data are also compared with small-angle neutron data on  $ZnBr_2$  aqueous and EtOAc solutions and the different structural properties induced by the different solvents are discussed.

**22.2-07** USE OF X-RAY ABSORPTION FOR DETERMINATION OF THE DENSITY OF SAMPLES IN STUDIES OF THE SCATTERING FROM FLUIDS.\* By M. Chandrasekhar, E. Gürmen\*\*, P.E. Chumbley, D.A. Dolejsi\*\*\*, H.D. Bale\*\*\*\*, and P.W. Schmidt, Physics Department, University of Missouri, Columbia, Missouri 65211 USA

Absorption of copper K- $\alpha$  X-rays has been used to determine the densities of the coexisting liquid and vapor phases of argon near the liquid-vapor critical point (150.7 K and 48 atm.). By an improvement of a technique developed previously [J.S. Lin and P.W. Schmidt, Phys. Rev. A 10, 2290-2304 (1974)], the densities of the two phases are calculated from measurements of the absorption along the 2-cm height of the vertical argon sample. While other, more conventional procedures give considerably higher precision than the 1 to 4 per cent possible with the absorption method, the X-ray technique permits determinations of the sample density under the same conditions that are used in small-angle X-ray scattering investigations [E. Gürmen, et al., Phys. Rev. A 22, 170-6 (1980)] and therefore is a convenient and reliable way of characterizing a sample being studied by scattering. The densities calculated from the absorption data are in good agreement with those which other investigators have determined by different techniques.

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**22.3-01** CHARACTERISATION OF SHORT RANGE ORDER IN AMORPHOUS AND LIQUID SYSTEMS. J. L. Finney\*, B. J. Gellatly\*, G. Bushnell-Wye\* and J. Wallace†. \* Crystallography Dept, Birkbeck College, Malet Street, London, WC1E 7HX, England. † Dept. of Physics and Astronomy, University College, Gower Street, London, WC1, England.

For the description of chemical ordering in models of metallic glass alloys, or for following local order changes on annealing, sensitive three-dimensional structural characterisation methods are necessary. We discuss here the merits or otherwise of three proposed methods.

(1) In the Voronoi polyhedron construction, the volume occupied by an N-atom model is partitioned into N non-arbitrary polyhedra, each containing all points in space closer to a given atom centre than to any other. The occurrence of certain polyhedron types has been used in discussing the validity of icosahedral models of single-component glasses (eg Barker et al, Nature 257, 1200 (1975)) and to identify crystalline nuclei (Tanemura et al, Prog. Theor. Phys. 58, 1079 (1977)). However, there is uncertainty in relating a given polyhedron type to a familiar real space structure, although the reverse procedure (real cluster to polyhedron) is fairly clear. Using an interactive computer graphics system, we have examined visually the polyhedra occurring in random packing glass models, and the changes in polyhedron topology consequent upon certain real space distortions followed. Some of the ambiguities observed in currently-made Voronoi real space identifications will be presented.

(2) The Radical Plane Polyhedron. As the Voronoi construction places dividing planes midway between atom centres, its application to assemblies of different-sized atoms results in dividing planes that intersect the bounding surfaces of the larger atoms. Too much volume is thereby allocated to the smaller component, too little to the larger and the polyhedron topology is liable to distortion. This problem is completely overcome by generalising the Voronoi procedure: the resulting radical plane construction (Fisher et al, Neues Jahrb. Min. Monat 227 (1971)) places the dividing plane in a position which takes account of the different radii yet remains rigorous. For touching or overlapping atoms, the plane is the common tangent and common chord respectively. Applications of the method to differently-constructed models of amorphous PdSi (Gaskell, J. Non-cryst Sol. 32, 207 (1979)) and FeB (Boudreaux and Gregor, J. Appl. Phys. 48, 5057 (1979)) will be described.

(3) Interstice Correlation Functions. Bernal (Proc. Roy. Soc. A 284, 299 (1964)) identified five types of "canonical hole" in hard sphere random packing; of these, the tetrahedron and octahedron were dominant (~75% by volume). In relaxed soft sphere models, however, the three other polyhedra are squeezed out, and it becomes possible to describe the assembly in terms of a packing of (distorted) tetrahedral and octahedral building blocks. A close-packed crystal structure can be described also as an assembly of the same building blocks, although more perfect and arranged in a regular, periodic manner. Thus if we regard the soft sphere random packing as an idealised glass, the possibility arises of a unified description of both non-crystalline and crystalline packed structures. Two aspects of such a possible description are discussed. First, partial correlation functions between like and unlike interstices indicate how the two types of building block are arranged in different glass models. Secondly, the power of a description of local ordering in terms of the arrangement of interstices about atom centres is compared to the much less sensitive Voronoi polyhedron approach.