22.X-01 NEUTRON SCATTERING, ISOTOPIC SUBSTITUTION AND THE STRUCTURE OF LIQUIDS AND AMORPHOUS SOLIDS. By

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The structure of liquids and amorphous solids are characterised by $\frac{1}{2}\nu(\nu+1)$ pair correlation functions where ν is the number of chemically distinct species. A single diffraction pattern contains an average over all the pair correlation functions whereas it is clear from a number of studies that critical tests of theory require knowledge of the individual pair correlation functions. The most successful method yet devised to extract these partial correlation functions is neutron diffraction combined with isotopic substitution. The technique will be illustrated by reference to recent studies on aqueous solutions, molten salts and liquid semiconductors. The characteristic short range order of each of these liquid types will be discussed and reference will be made to current theoretical developments.

22.1-01 INVESTIGATION OF LIQUID CRYSTALS IN THE HIGH VOLTAGE ELECTRON MICROSCOPE.

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Since direct electron microscopic transmission of liquid crystals is chiefly limited by vapour pressure and beam damage problems, few results are known up to now. This paper shows that high voltage electron microscopy - due to its lower ionization damage - is a successful tool for imaging structural details below the textures known from optical microscopy and to obtain diffraction from single crystalline specimen regions of ≈ 10 µm diam. Substances of low vapour pressure, e.g. thermotropic smectic phases, can be transmitted without use of specimen capsules.
Thin-film specimens of 4-n-hexyloxy-4'-n-hexylbiphenyl up to 4 µm thickness (prepared by vacuum deposition and optically tested) were transmitted at 1000 kV. They exhibit single crystalline grains of ≈ 10 µm diam. Electron diffraction reflections satisfy $(h + k + l) = 2n$ due to an orthorhombic unit cell orientated with the smectic layers parallel to the film plane. The latter condition may restrict the variety of possible textures. Inside the grains, diffraction contrast reveals certain types of dislocation lines that can be attributed to mutual displacement of parallel layers.
Radiation damage at doses above $3 \cdot 10^{-2}$ As/cm^2 causes growth of bubbles disturbing fine image details whereas the diffraction pattern remains much more stable.

22.1-02 ORIENTATIONAL-DISORDER MODELS FOR LIQUID CRYSTAL PHASES.

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In a first approximation, most liquid crystal molecules may be considered as cylindrical rods. The basic feature governing the packing of such molecules is that the long axes of adjacent rods are more or less parallel to each other. It has, of course, always been known that these axes are never exactly parallel, and that there is always a certain amount of orientational disorder, but it appears that certain aspects of this disorder have not been adequately taken into account.

Recently, we have shown that many long-standing discrepancies, between measured layer thicknesses of smectic phases and the lengths of the molecules in these layers, can be simply explained by taking account of the orientational disorder (A. de Vries, A. Ekachai, and N. Spielberg, Mol. Cryst. Liq. Cryst. Lett. (1979) 49, 143). For the smectic A phase, e.g., the directions of the long molecular axes are distributed over a diffuse cone, with infinite rotational symmetry, around the normal to the smectic layer. This results in an "orthogonal" phase, i.e., a phase in which the average direction of the long axes is perpendicular to the layer plane. With such a model for an orthogonal phase, there are two different models possible for a "tilted" phase: the "tilted-cone" model and the "asymmetric-cone" model (A. de Vries, Proceedings of the Third Liquid Crystal Conference of Socialist Countries, Budapest, Hungary, 1979). The tilted-cone model is obtained, from the symmetric-cone model of the smectic A phase, by tilting the cone axis away from the layer normal. The asymmetric-cone model is obtained from the symmetric-cone model by leaving the cone axis perpendicular to the layer plane, but introducing a certain asymmetry in the distribution of the directions around this axis, retaining only the symmetry of a mirror plane through the cone axis and the tilt direction.

For a well-defined layer structure, the asymmetric-cone model appears to be more appropriate than the tilted-cone model. The asymmetric-cone model has been used, therefore, to describe the smectic C phase (A. de Vries, J. Chem. Phys. (1979) 71, 25). The tilted-cone model, on the other hand, would seem more suitable for phases with very weak smectic order, e.g., for the skewed cybotactic nematic phase. Attempts to fit this model--or any other cone model--to recently obtained accurate and extensive data on the layer thickness and the tilt angle in a series of skewed cybotactic nematic phases (V.M. Sethna, A. de Vries, and N. Spielberg, Mol. Cryst. Liq. Cryst. (1980) 62, 141), however, did not succeed until after the introduction of the following modification. It was realized that the local order, in a cybotactic group, is not necessarily the same as the overall order in the sample. Thus, in fitting the tilted-cone model to the data, we allowed the local director to make an angle with the overall director, and we allowed the local orientational order parameter to be different from the overall orientational order parameter (V.M. Sethna, Ph.D. Dissertation, Kent State University, USA, 1980). The fits obtained with this "conical tilted-cone" model were excellent. The differences between the two order parameters were only relatively small, and the local order was always greater than the overall order, as would be expected. The way in which the various model parameters varied as function of temperature suggests that the conical tilted-cone model applies not only to the skewed cybotactic nematic phase but also the ordinary nematic phase.