22. GASES, LIQUIDS AND AMORPHOUS COMPOUNDS

22.1-1 THE GENERALIZED CRYSTALLOGRAPHY.

By R. Hosemann, Gruppe Parakkristalforschung, c/o BAM, Kantilenstraße 21, Berlin 45, Germany.

The well-known intensity function $I(b) = 1/\lambda f^2 S^2$ of the kinematic scattering of a crystal reported by Boz (London), (1940) 22, 167, was generalized in 1950 to the so-called ideal paracrystal (Hosemann, Z. Phys. (1965) 278, 465).

Holland's peak function $I(b)$ was replaced by the Fourier transform of a convolution polynomial which depends on at least nine parameters $g_{ik}(1k=1,2,3)$ which define liquid-like relative distance variances of adjacent lattice bricks. The shape factor of a paracrystal with $N$-netplanes in the direction $L$ is related to the value $g_L$ by $g_L = \alpha^L$. In 20 years of systematic work this formula has been experimentally confirmed for real microparacrystals with a value $\alpha^L \approx 1 - 0.05$, including matter ranging from melts with values $g_L \approx 0,0$ up to catalysts with $g_L \approx 0.01$.

Just recently statistical methods led to the proof that there exists a $\alpha_L$-conducted equilibrium state where the $\alpha_L$-relation defines the average number of netplanes in an ensemble of microparacrystals (Hosemann et al., Colloid and Polymer Sci. (1981) 259, 116). A novel tangential intermolecular potential energy $\phi_A$ plays the dominant role and leads to the free enthalpy $AG$ given for cubic microparacrystals by $AG = N^H + N^D + N^A g_{ik}$ from the line profile- and ESR-experiments two further direct evidences were obtained which confirm the reality of this new kind of equilibrium state (Hindeleh, Hosemann, Polymer (1982) 23, 110) and the fundamental importance of the $\alpha_L$-relation for all colloids (Hosemann, Colloid and Polymer Sci. (1982) 260, 864).

22.1-2 THE GENERALIZED FOURIERTRANSFORM

By R. Hosemann, Gruppe Parakkristalforschung, c/o BAM, Kantilenstraße 21, Berlin 45, Germany.

Critical scattering of X-rays in a liquid crystal at temperatures above a phase transition point is caused by fluctuations of the corresponding low-temperature phase. Critical scattering data therefore could reveal the symmetry of the low-temperature phase if a scattering cross-section having the same symmetry of that phase, were available. A method of calculating critical scattering cross-sections with the point-group symmetry of the scattering system /J. Kocinski, Theory of Symmetry Changes at Continuous Phase Transitions, Elsevier 1983/ has been applied to liquid crystals. This method consists in constructing a correlation function, which is invariant under the symmetry operations of the relevant point group, whose Fourier transform yields a cross-section with the same symmetry. Critical scattering cross-sections with 6/mmm and 00/2mm symmetries have been determined. They enable the interpretation of the constant scattered intensity curves which have been determined by critical X-ray scattering in DHB amic at the phase transition ammic $B \rightarrow$ isotropic liquid.

22.1-3 X-RAY STUDY OF PHASE TRANSITION IN HEXACHLOROETHANE.

By T. Pura and J. Piredo, Polish Inst. of Physics, Warsaw Technical University, Koszykowa 75, 00-662 Warszawa, Poland.

The high temperature phases of numerous molecular crystals are characterized by orientational disorder. Scattering patterns taken in these so-called plastic phases show only a few Bragg reflections superimposed on a strong continuum of diffuse scattering. We demonstrate using the example of hexachloroethane how the analysis of diffuse X-ray scattering in highly disordered systems can give corresponding and complementary information to a conventional structure determination using Bragg intensities. The work is divided into two parts.

A model structure generated by a Monte Carlo method is compared with the experimental data. The Fourier-transformed one-particle model scattering density describes very well the diffuse patterns coming from uncorrelated disordered molecules. By this simulation we demonstrate clearly the influence of the hard core repulsive force considered in the model on the rotational-translational distribution of the molecules.

Futhermore, the existence of a one-dimensional short range orientational order is proved. The corresponding planes of diffuse intensity can be described by using an extended ising model for the orientation, which has several possible directions.

22.1-4 AN ANALYSIS OF THE DIFFUSE X-RAY SCATTERING IN THE ORIENTATIONALLY DISORDERED PHASE OF HEXACHLOROETHANE.


The well-known intensity function $I(b) = 1/\lambda f^2 S^2$ of the kinematic scattering of a crystal reported by Boz (London), (1940) 22, 167, was generalized in 1950 to the so-called ideal paracrystal (Hosemann, Z. Phys. (1965) 278, 465).

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Just recently statistical methods led to the proof that there exists a $\alpha_L$-conducted equilibrium state where the $\alpha_L$-relation defines the average number of netplanes in an ensemble of microparacrystals (Hosemann et al., Colloid and Polymer Sci. (1981) 259, 116). A novel tangential intermolecular potential energy $\phi_A$ plays the dominant role and leads to the free enthalpy $AG$ given for cubic microparacrystals by $AG = N^H + N^D + N^A g_{ik}$ from the line profile- and ESR-experiments two further direct evidences were obtained which confirm the reality of this new kind of equilibrium state (Hindeleh, Hosemann, Polymer (1982) 23, 110) and the fundamental importance of the $\alpha_L$-relation for all colloids (Hosemann, Colloid and Polymer Sci. (1982) 260, 864).

The liquid crystal of $\text{C}_2\text{H}_{4}\text{Cl}_2 = \text{CCl}_2\text{COO} = \text{CCl}_2\text{CN}$ has been investigated by ISC, by polarisation microscopy and by X-ray diffraction. The following phase diagram has been determined:

Cr $\rightarrow$ N $\rightarrow$ $\phi_\text{re}$ $\rightarrow$ N $\rightarrow$ $\phi_\text{re}$ $\rightarrow$ Iso

The samples have been oriented in magnetic fields, experiments have been performed with the use of photographic and spectrometric method. In the Sm$^*$ state a single peak with wave vector $q_1 = 0.56 \text{ Å}^{-1}$ has been observed while in N$\rightarrow$ phase two sharp peaks $q_2 = 0.12 \text{ Å}^{-1}$ and $q_3 = 0.18 \text{ Å}^{-1}$ at 110°C have been detected. The measurements of X-ray critical scattering near the $\phi_\text{re}$ phase transition have been carried out on two crystal spectrometers with the use of Cu radiation monochromatized with help of $\phi_\text{re}$ Ge flat crystals. The longitudinal $\phi_\text{re}$ and transverse $\phi_\text{re}$ correlation lengths $\xi \rightarrow 0$ for $T = 2.5 \phi_\text{re}$ temperature behaviour of the intensity of the peaks has been measured in the N, $\phi_\text{re}$ and $\phi_\text{re}$ temperature range.