

22.1-5 CRYSTALLOGRAPHIC STUDY OF SODIUM DECYL SULPHATE, By D.R.Bittencourt and L.Q.Amaral, Instituto de Física, University of São Paulo, São Paulo, Brasil.

The system Na decyl sulphate (SDS)/water/additives (salt and/or alcohol) form nematic lyomesophases ( $N_L$  with disc micelles and  $N_C$  with cylindrical micelles) above and coagel G mesophases below the Krafft melting temperature of the hydrocarbon chains. It has been proposed that in nematic phases micelles are not homogeneously dispersed in water but aggregates are formed (Amaral & Figueiredo, Mol.Cryst.Liq.Cryst. (1983)98,285; Acta Cryst. (1983)A39, 651). It was considered important to obtain crystallographic data of the amphiphile pure to compare with diffraction results in N and G phases, since no such data exist in the literature. Good quality SDS monocrystals are difficult to obtain and therefore a crystallographic study of SDS in powder form was performed. SDS density was measured by the picnometer method (with collaboration of H.Murakawa) resulting  $(1.222 \pm 0.004) \text{g/cm}^3$  at 20°C. Indexing of the reflections has been made considering known diffraction patterns of odd paraffins (Doucet et al, J. Chem.Phys. (1981)75,1523) and also the Ito method. The proposed unit cell is monoclinic with parameters  $a=(8.23 \pm 0.02) \text{Å}$ ,  $b=(5.11 \pm 0.02) \text{Å}$ ,  $c=(34.2 \pm 0.15) \text{Å}$  and  $\beta=(97.1 \pm 0.3)^\circ$ . No extinctions indicate as probable spacial groups  $P_2$ ,  $P_m$  or  $P_{2/m}$ . An attempt to determine the structure from monocrystals is under course. The results obtained with powder can already be used to extract information about the aggregates of the G and N phases. The lamellar repetition distance of the G phase is  $31.1 \text{Å}$ , smaller than that of the amphiphile; this shows that the aggregates are most probably anhydrous and with a tilt angle. This result in turn allow a better prediction of the expected lamellar thickness for the nematic phase. As diffraction bands in N phases occur at 38-39 Å, little space is left for water, which constitutes 53% of the system; this supports the model of aggregates for N phases.

22.1-6 KINETIC PHASE CHANGES IN LIQUIDCRYSTALLINE MEDIA. By E.V.Kononenko. Ural Polytechnical Institute, 620002 Sverdlovsk-2, USSR

In a number of cases the structural changes and the crystal growth (CG) from liquidcrystalline (LC) media can be considered as kinetic phase changes with anisotropic kinetic factors. Crystallographic parameters depend essentially on the orientation on the substrate, the flow directions in the capillar and imperfections playing a role in the temperature factor. Dislocation-disclination (DD) mechanisms of the transition nematic - cholesteric in plane capillars with the concentration gradient are studied. The wave-like instability (I) effect established is described in terms of the DD-transformations. The development and relaxation kinetics of I indicates that there are certain boundary conditions and the capillar thickness range at which the I-effect is possible at the fixed original pitch of the cholesteric. The peculiarities of CG from multicomponent stable and non-equilibrium layered LC phases are analysed in terms of the elasticity theory, DD approach and the kinetic phase changes. It is established that at isothermal conditions the CG mechanisms, the shape and morphology of crystals are determined by the orientation on the substrate and by the relation between the capillar thickness and that of the uniformly oriented layer. It is supposed that x-disclinations are the main defects at the dislocational CG in the cholesteric LC phase.

22.1-7 MOLECULAR MOTION AND CONFORMATIONAL DEFECTS IN ODD-NUMBERED PARAFFINS.

By A.F. Craievich (1), I. Denicolo (2) and J. Doucet (3). (1) LURE, Université Paris-Sud, Orsay, France and CNPq/CBPF - Rua Dr. Xavier Sigaud, 150-22290 Rio de Janeiro, RJ, Brasil. (2) Departamento de Física, UFSC, 88000-Florianópolis, SC, Brasil. (3) Laboratoire de Physique des Solides, Université Paris-Sud, Bât.510, 91405 Orsay, France.

The paraffins  $C_n H_{2n+2}$  with n ranging from 9 to 40 exhibit an intermediate phase, called rotator phase, between the crystalline and liquid phases. The rotator phase is characterized by a layered structure in which the molecules, which are oriented perpendicularly or slightly tilted to the layers, undergo reorientational motions around their long axis. In addition to this motion, longitudinal molecular motions and conformational defects have been recently detected; by small angle X-ray diffraction studies using synchrotron radiation we intended to precise their magnitude, both as a function of n ( $19 \leq n \leq 27$ ) and temperature. In short, the molecular conformational defects are mainly formed at the transition crystal  $\rightarrow$  rotator temperature and their concentration increases with n. The longitudinal molecular motion greatly increases at the transition crystal  $\rightarrow$  rotator temperature and its amplitude increases both with n and temperature. The amplitude of the longitudinal molecular displacements and the defect concentration are correlated.

22.1-8 PHASE TRANSITIONS IN ORIENTATIONALY ORDERED SYSTEMS OF ASYMMETRIC AND SEMI-FLEXIBLE MOLECULES. By V.I.K.Pershin and V.A.Konoplev. Ural Polytechnical Institute, 620002 Sverdlovsk-2, USSR.

The aim of the paper is the theoretical investigation of effects of the molecules asymmetry and semi-flexibility on phase transitions (PT) in orientationally ordered systems (liquid crystals, n-alkanes, lipids e.a.). In terms of the variational approach the dynamic equations for local orientational fluctuations of asymmetric rigid semi-flexible molecules of different length are obtained. It is shown that the structural PT bound with the anomalous behaviour of the mean-square particles displacements in the vicinity of the instability point takes place. It is established that the negative asymmetry promoting the molecules packing of "head-to-tail" type destabilize orientational order in the system and the positive asymmetry is quite the reverse. For the case of semi-flexible molecules it is shown that besides of the transition into the disordered state the structural transformations leading to partially ordered phases with more developed orientational and conformational disorder may occur depending on the degree of molecular flexibility and anisotropy. The conditions of the realization of PT occurring without the symmetry change and those of the reentrant type are found. The results are compared to known experimental data for liquid crystals, paraffins and lipids. The regimes not observed earlier are predicted in the behaviour of the systems of asymmetric and semi-flexible molecules.