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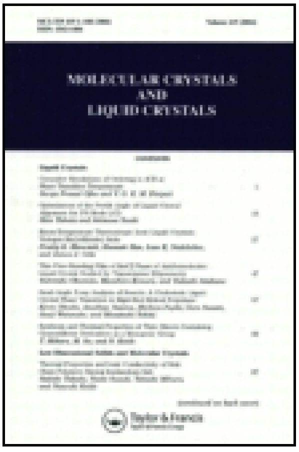

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Flowability and Crystal Order. Smectic B Model

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FLOWABILITY AND CRYSTAL ORDER. SMECTIC B MODEL

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Abstract A model of smectic B liquid crystal (Sm B) is suggested. According to this model Sm B is characterized by crystal translational order in all directions. At the same time interlayer shear modulus C_{1313} decreases at lower frequencies of external effect ω_{ex} and equals zero in the static case ($\omega_{ex} \to 0$). The model is based on the account of terms nonlinear with respect to wave vector $\vec{K}$ in the frequencies of translational oscillations.

FORMALISM AND MODEL

It has been shown [1,2] that elastic energy connected with shear of the layers parallel to each other is

$$F_{in} = \frac{C_{1313}}{2}\left[\left(\frac{\partial U_x}{\partial z}\right)^2 + \left(\frac{\partial U_y}{\partial z}\right)^2\right] + \frac{K_{33}}{2}\left[\left(\frac{\partial^2 U_x}{\partial Z^2}\right)^2 + \left(\frac{\partial^2 U_y}{\partial Z^2}\right)^2\right]. \quad (1)$$

It has been found that

$$C_{3131} - C_{1313} = \frac{\partial^2 F_{or}}{\partial n_x^2} > 0. \quad (2)$$

Here U_x and U_y are displacements from equilibrium position within the layer, U_z is displacement normal to the layers, K_{33} is Frank-constant, F_{or} is energy of orientational deformations, $\vec{n}$ is director ($\langle \vec{n} \rangle = \{0,0,1\}$). It has been estimated that $C_{3131} - C_{1313} \sim \sim 10^8$ dyn/cm^2. This result corresponds to experimental data[3]. Using (1) and (2) translational oscillation frequencies (ω_i) have been obtained

$$\rho\omega_1^2 = C_{11} K^2 + C_{1313} K_z^2 + K_{33} K_z^4 ; \qquad (3)$$

$$\rho\omega_2^2 = C_{66} K^2 + C_{1313} K_z^2 + K_{33} K_z^4 ; \qquad (4)$$

$$\rho\omega_3^2 = C_{3131} K^2 + C_{33} K_z^2 . \qquad (5)$$

Ratio (2) and account of nonlinear terms (i.e. proportional to K_z^4) in the frequencies (3),(4) determine the specific features of the system in question.

We have got

$$\langle U_z^2 \rangle = \frac{8T}{\pi^3 M} \int_0^{\pi/2} \omega_3^{-2}\, d^3\theta ; \qquad (6)$$

$$X(L_3) = \frac{32T}{\pi^3 M} \int_0^{\pi/2} (\omega_1^{-2} + \omega_2^{-2}) \sin^2(K_z L_3/2)\, d^3\theta ; \qquad (7)$$

$$\langle U^2 \rangle = \frac{8T}{\pi^3 M} \int_0^{\pi/2} (\omega_1^{-2} + \omega_2^{-2})\, d^3\theta , \qquad (8)$$

$$\langle U^2 \rangle = \langle U_x^2 \rangle + \langle U_y^2 \rangle ,$$

where T is temperature; $\theta_x = K_x l/2$; $\theta_y = K_y l/2$; $\theta_z = K_z l_3/2$; l is lattice spacing; l_3 is layer spacing; $X(L_3) = \langle [U_x(0) - U_x(L_3)]^2 \rangle + \langle [U_y(0) - U_y(L_3)]^2 \rangle$; $L_3 = l_3 P$; $P = 1,2,3,\ldots$; M is molecule mass.

The state when interlayer shear modulus $C_{1313} = 0$, while all other coefficients in the frequencies (3) - (5) are other than zero is treated as smectic B model.

ELASTIC PROPERTIES

It follows from (2) that due to the presence of orien-

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tational order Sm B is stable relative to the bend of the layers $C_{3131} \neq 0$.

Let us analyse system stability relative to the shear of the layers parallel to each other. It is clear from (1) that in the case $C_{1313} = 0$, $K_{33} \neq 0$ the system is unstable relative to linear$(\partial^2 U_i/\partial z^2 = 0;$ $i = x,y)$ deformations $F_{in}(U_i = 0) = F_{in}(U_i = P_i z)(P_i = \text{const})$. Nonlinear deformations $(\partial^2 U_i/\partial z^2 \neq 0)$ lead to larger elastic energy, i.e. cause the appearance of restoring forces. It is clear that such deformations take place if external effect is time-dependent.

To get quantitative description of"nonlinear" restoring forces from (1),(3),(4) effective interlayer shear modulus can be introduced

$$C^{ef}_{1313} = K_{33} K_z^2 = (\rho K_{33})^{1/2} \omega_{ex} \, . \tag{9}$$

We can see from this expression that the system is unstable relative to static linear deformations. However, due to nonlinear effects interlayer shear modulus becomes other than zero in the case of nonlinear deformations (e.g. dynamical). It becomes larger if "nonlinearity" K_z^2 (or frequency of external effect ω_{ex}) increases. $K_{33} \approx 3{,}4 \cdot 10^{-2}$dyn has been estimated for Sm B compound 40.8 ($C^{ef}_{1313} = 1.7 \cdot 10^7$dyn/cm^2 if $\omega_{ex}/2\pi = 15$ MHz [4]).

TRANSLATIONAL ORDER

Integrating (6) and accounting for $C_{33} \gg C_{3131}$ ($C_{33} \approx 1.2 \cdot 10^{10}$dyn/cm^2 [3], $C_{3131} \approx 10^8$dyn/cm^2, $T/k = 400$ K) we can obtain $\sqrt{\langle U_z^2 \rangle} \approx 1.6$ Å $\ll l_3$. This result agrees to experimental data[5] and proves that there is long-range translational order in the direction normal to the layers.

It follows from (7) and (8) that i) layers are correlated, i.e. $\exp\left[-2\pi^2 X(L_3)/l_3^2\right] \to \text{const} \neq 0$ if $L_3 \to \infty$; ii) there is long-range translational order within the layer, i.e. $\sqrt{\langle U^2\rangle} \approx 0.3$ Å $\ll 1$ ($C_{11} \approx 2.6 \cdot 10^{10}$ dyn/cm^2; $C_{66} \approx 4.9 \cdot 10^9$ dyn/cm^2 [3]). This value $\sqrt{\langle U^2\rangle}$ corresponds to the experimental data [5].

We get that crystal order can coexist with static shear instability. This result is based on the account of nonlinear effects. If $C_{1313} = 0$, then nonlinear terms are responsible for the convergence of integrals (7),(8). It means that "nonlinear" restoring forces cause interlayer correlations and stabilize 3-dimensional crystal order within the layer.

CRYSTAL - Sm B PHASE TRANSITION

It has been concluded that entropy jump ΔS_{CB} is not determined by the changes of system ordering. ΔS_{CB} is connected with the change of elastic moduli

$$\Delta S_{CB} = C \ln\left[C_{33}(Cr)/C_{33}(B)\right]. \tag{10}$$

where C is heat capacity, $C_{33}(Cr)$ and $C_{33}(B)$ are elastic moduli in the crystal and Sm B, respectively. Estimates give reasonable value of $\Delta S_{CB} = 18$ cal/mole·K ($C_{33}(Cr)/C_{33}(B) \approx 1.17$ [3]).

CONCLUSION

The suggested "nonlinear" Sm B model explains the following experimental data[6,7,8] : 1.Change of dispersion curve of transverse wave at the crystal-smectic B

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transition when the wave propagates normally to the layers (in Sm B it closely resembles a parabola $\omega \sim K_z^2$) 2. C_{1313} decreases at lower frequencies ω_{ex}. 3. C_{1313} equals zero in the static case ($\omega_{ex} \to 0$). These results cannot presumably be explained in terms of "crystalline" model[9] of Sm B.

It should be noted that the main idea of this paper (nonlinear effects should be accounted for if shear moduli are equal to zero) has been used by the authors[1,2] when they studied translational correlations and elastic properties in partially ordered smectic phases.

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