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SURFACE-INDUCED ORDER PARAMETER PROFILES IN A NEMATIC LIQUID CRYSTAL FROM MOLECULAR DYNAMICS SIMULATIONS

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Abstract The tensor order parameter of a model nematic liquid crystal close to a rough surface has been analyzed by means of molecular dynamics simulations. We show that the rough surface induces a smectic C layering. Moving towards the bulk, the smectic order disappears and a depression in the uniaxial orientational order below its bulk value occurs, accompanied by a considerable biaxiality. Correspondingly, the director orientation undergoes a strong distortion localized within a few molecular lengths.

Elastic distortions in the bulk director field $\mathbf{n}$ of nematic liquid crystals occur on a macroscopic scale and are well-described in terms of the Oseen-Zöcher-Frank elastic theory. Close to a surface, however, additional contributions become important[1]. Among these, the K_{13} constant, giving the energy density $K_{13}\ \mathrm{div}(\mathbf{n}\ \mathrm{div}\,\mathbf{n})$, poses severe mathematical problems, since it makes the total elastic energy of a distorted sample unbounded from below. Various approaches have been suggested to overcome this problem. One of the solutions gives rise to strong distortions localized on a molecular dimension close to the surface[2]. This conclusion has been opposed by some other authors, who claim that such subsurface deformations are an artifact of the low-order elastic theory[3]. All these descriptions rely on continuum theories that are strictly valid only on a macroscopic level. Therefore, a proper investigation of a possible existence of a subsurface deformation should be based on a molecular approach.

In order to investigate the structural changes in a nematic liquid crystal close to a rough surface we have performed molecular dynamics simulations. The molecular pair interactions in the bulk were evaluated from the Gay-Berne potential[4]. The phase diagram for this model is well-established, and the surface elastic constant K_{13} has been evaluated to be non-zero. The surface was modeled by assuming

a one-dimensional Lennard-Jones potential for the dependence on the molecular distance along the surface normal (z-axis). The orienting properties of the surface were taken into account by an anisotropic ground state energy, that favors molecular alignment along an easy direction $\mathbf{k}$

$$V_{\text{surf}} = 4\,\epsilon_{\text{surf}}\left[1 + \chi^2_{\text{surf}}\,(\mathbf{e}_i \cdot \mathbf{k})^2\right] \cdot \left[\left(\frac{\sigma_0}{z - z_{\text{surf}}}\right)^{12} - \left(\frac{\sigma_0}{z - z_{\text{surf}}}\right)^{6}\right], \qquad (1)$$

where ϵ_{surf} measures the strength of the surface potential and χ_{surf} its anisotropy.

In order to describe a rough interface we used a surface sinusoidally modulated in the lateral dimensions: $z_{\text{surf}} = z_0 + a\,\sin(k_x x)\,\sin(k_y y)$. For the analysis of surface-induced ordering the time-averaged z-profiles of the particle density and the nematic tensor order parameter $\mathbf{Q}$ were evaluated. In order to obtain a smooth profile, the $\mathbf{Q}$ tensor was calculated as an average over all molecular orientations $\mathbf{e}_i$, multiplied by a Gaussian weight for the molecular positions z_i

$$\mathbf{Q}(z) = \overline{\langle\left[\frac{3}{2}\,\mathbf{e}_i \otimes \mathbf{e}_i - \frac{1}{2}\right] \exp\left(-\frac{(z - z_i)^2}{2\sigma^2}\right)\rangle}\,.$$

By a diagonalization of the tensor order parameter, the uniaxial scalar order parameter $S(z)$ and the biaxial one $P(z)$ were extracted from the tensor eigenvalues $-\frac{1}{2}S + \frac{1}{2}P$, $-\frac{1}{2}S - \frac{1}{2}P$, S, whereas the orientation of the main director $\mathbf{n}(z)$ was determined as the eigenvector belonging to the largest eigenvalue S.

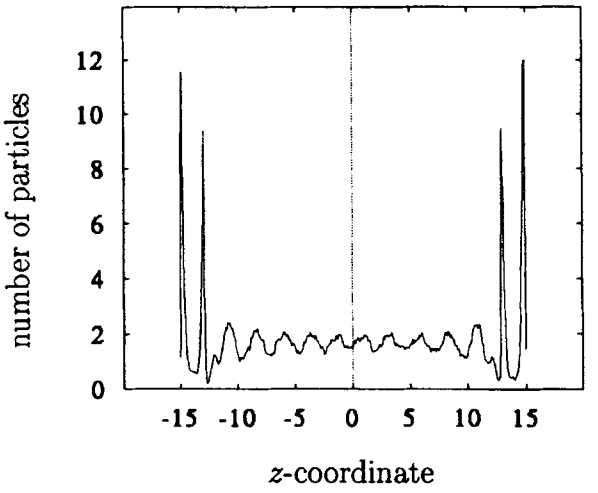

FIGURE 1 z-profile of the particle density (surface easy axis $\theta_p = 70°$).

Fig. 1 shows the density profile along the surface normal z. Close to each surface ($z = \pm 15$) there are two smectic C layers (surface easy axis $\theta_p = 70°$) that

correspond to the hills and valleys of the undulated surface. In the bulk there is hardly any positional order.

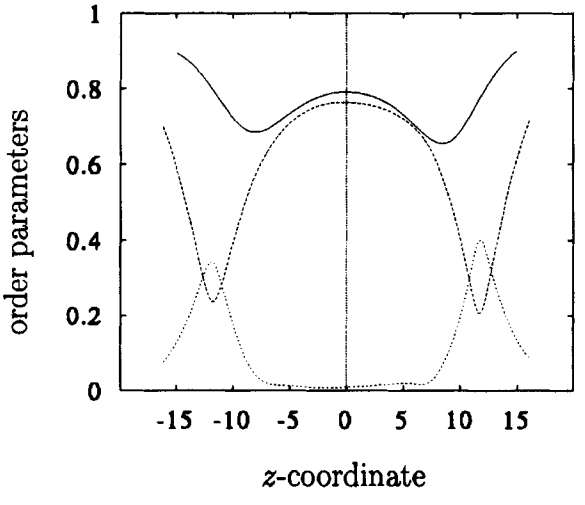

FIGURE 2 z-profile of the orientational order parameters. Solid line: $S(\theta_p = 20°)$, dashed line: $S(\theta_p = 70°)$, dotted line: $P(\theta_p = 70°)$.

The z-profiles of the orientational order are displayed in Fig. 2. On the surfaces the uniaxial order is very high: the molecules in the smectic layers are mostly oriented along the easy axis. In the bulk ($z = 0$) we find $S = 0.7 - 0.8$, typical for the Gay-Berne model. Most interestingly, between the surface and the bulk there is a region where the uniaxial order is strongly depressed. Additionally, the biaxial order parameter P takes values that are significantly non-zero in this region.

Such changes in the orientational order are accompanied by a strong deformation in the director orientation. Fig. 3 reveals the z-profile of the director tilt angle $\theta(z)$ for two surface pretilts ($\theta_p = 20°$ and $\theta_p = 70°$). On the surfaces the director points along the easy axis, moving towards the bulk there is a strong distortion to an almost homeotropic orientation.

Recent investigations showed that the distorting effect of the Gay-Berne potential (connected with the non-vanishing surface elastic constant K_{13}) favors a homeotropic alignment. Our analysis reveals, however, that smectic layers and biaxiality, as well as the gradients of the uniaxial order, play an important rôle close to the surface.

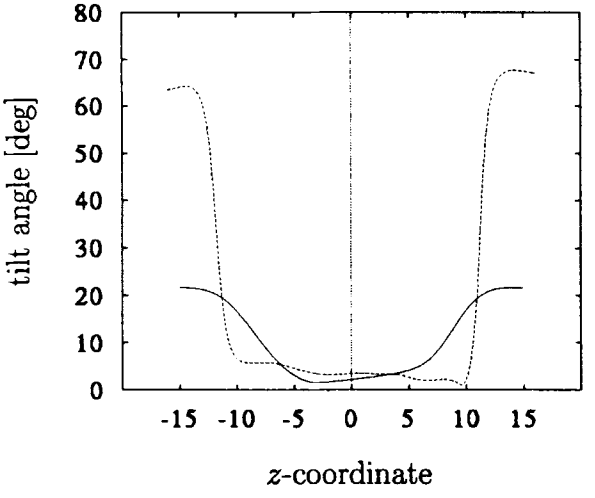

FIGURE 3 Tilt angle profile $\theta(z)$. Solid line: surface easy axis $\theta_p = 20°$, dashed line: surface easy axis $\theta_p = 70°$.

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