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Anchoring of a nematic liquid crystal induced by surface grooves: A numerical study

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To examine the anchoring energy of a surface with one-dimensional grooves of sinusoidal shape, we carry out numerical calculation of the Frank elastic energy of a nematic cell composed of such a grooved surface and a flat surface. We evaluate the anchoring energy of the grooved surface by carefully eliminating the contribution from a uniform twist deformation in the bulk. When $qA \lesssim 0.2$, with q and A being the wave number and the amplitude of the surface groove, we find that the azimuthal-angle dependence of the calculated anchoring energy agrees perfectly with our previous analytical result under the assumption of $qA \ll 1$ [Fukuda *et al.*, Phys. Rev. Lett. **98**, 187803 (2007); **99**, 139902(E) (2007)]. Even when $qA \simeq 0.6$ or 1, we observe an unexpectedly good agreement between the calculated and the analytical anchoring energies, indicating the wide applicability of the analytical anchoring energy in spite of the assumption of $qA \ll 1$ in its derivation.

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Surface anchoring [1,2] is one of the most important properties of liquid crystals, mainly because of its relevance in practical applications such as liquid crystal displays. Recently, there have been many experimental attempts [3–6] to achieve some desirable anchoring properties by surfaces tailored with microscopic grooves or geometrical patterns. Those studies have been attracting attention because they propose novel methods of preparing anchoring surfaces different from conventional techniques such as surface rubbing.

Theoretical studies to elucidate the anchoring properties of such microscopically grooved surfaces can date back to the well-known pioneering study of Berreman [7]. In our recent studies [8–10], however, we revealed that Berreman's study is insufficient in that it was based on an invalid assumption of no azimuthal director distortions and did not incorporate the effect of surfacelike elasticity. We gave a rigorous analytic formula of azimuthal anchoring energy of a nematic liquid crystal for surfaces with one-dimensional parallel grooves [8,9], or ones with arbitrary patterns [10]. However, our analytic argument, as well as Berreman's original one, is based on an assumption that the surface slope is small enough; otherwise the nonlinear nature of the Frank elastic energy does not allow one to carry out purely analytic argument. Therefore numerical studies will be inevitable to understand the anchoring properties of grooved surfaces with relatively large slopes. Although there have been several numerical attempts [11–13] to investigate how a nematic liquid crystal behaves in the vicinity of a grooved surface, none of them aimed at the evaluation of the anchoring energies of such surfaces. The purpose of the present study is to perform numerical calculations to evaluate the anchoring energy of one-dimensionally grooved surfaces and to find out how much our previous analytical argument is applicable.

The free energy density of a nematic liquid crystal is given by the Frank elastic energy density that is written in terms of the director $\boldsymbol{n}$ ($|\boldsymbol{n}|=1$) as [1,14,15]

$$f_{\mathrm{Frank}}\{\boldsymbol{n},\nabla\boldsymbol{n}\} = \frac{1}{2}\{K_1(\nabla\cdot\boldsymbol{n})^2 + K_2(\boldsymbol{n}\cdot\nabla\times\boldsymbol{n})^2 + K_3(\boldsymbol{n}\times\nabla\times\boldsymbol{n})^2 - K_s\nabla\cdot(\boldsymbol{n}\nabla\cdot\boldsymbol{n}+\boldsymbol{n}\times\nabla\times\boldsymbol{n})\}, \quad (1)$$

where K_1, K_2, and K_3 are the bulk elastic constants associated with splay, twist, and bend deformations, respectively. The last term in Eq. (1) is referred to as a surfacelike elastic term because it is converted to a surface integral. We have introduced $K_s \equiv K_2 + K_{24}$, where K_{24} is the saddle-splay elastic constant [14–16]. Another surfacelike term involving K_{13} is not considered here [17].

We consider a surface with one-dimensional (1D) parallel grooves along the y direction and assume uniformity along this direction ($\partial/\partial y = 0$). The height of the surface with respect to a reference plane, $z=0$, is assumed to be given by a sinusoidal function $h(x)=A\sin qx$. Here q and A characterize the pitch and the amplitude of the surface grooves, respectively. At this lower surface, we assume that the director $\boldsymbol{n}$ is always tangential to the surface and no preferred direction is present. This boundary condition is simply written as $\boldsymbol{n}\cdot\boldsymbol{\nu}=0$, with $\boldsymbol{\nu}$ being the surface normal. This assumption is exactly the same as that employed in our previous analytic studies [8,9].

We also introduce an upper plane surface, $z=L_z$, where we fix the director as $\boldsymbol{n}=(\cos\phi,\sin\phi,0)$. We calculate the total free energy of the system for various ϕ to examine the azimuthal angle dependence of the anchoring energy. We note that due to the treatments above, we do not have surface free energies for the upper and lower surfaces, and thus the total free energy of the system is given solely by the Frank elastic energy, Eq. (1).

In our numerical system, we assume a periodic boundary condition along the x direction, so that the director profile satisfies $\boldsymbol{n}(x,z)=\boldsymbol{n}(x+mL_x,z)$, with m being an arbitrary integer. The period L_x must conform to the periodicity of the

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surface, and thus we set $L_x=2\pi/q$. The area of our numerical system in the (x,z) space is described by $0\leqslant x<L_x$ and $h(x)\leqslant z\leqslant L_z$.

After introducing a variable $\zeta(x,z)$ satisfying $z=\zeta+(1-\zeta/L_z)h(x)$, our system is mapped onto a rectangle in the (x,ζ) space: $0\leqslant x<L_x$ and $0\leqslant\zeta\leqslant L_z$. The total free energy per unit area of the surface is then given by

$$F=\frac{1}{L_x}\int_0^{L_x}dx\int_0^{L_z}d\zeta\frac{\partial z}{\partial\zeta}f_{\mathrm{Frank}}\{\boldsymbol{n},\partial_x\boldsymbol{n}(x,\zeta),\partial_\zeta\boldsymbol{n}(x,\zeta)\}. \quad (2)$$

We discretize the rectangle in the (x,ζ) space by $N\times(N+1)$ grid points with equal grid spacings. In the present calculations, we choose $N=32$. The values of the director $\boldsymbol{n}$ are assigned at each grid point as $\boldsymbol{n}_{i,k}=\boldsymbol{n}(x=i\Delta x,\zeta=k\Delta\zeta)$, with $\Delta x\equiv L_x/N$, $\Delta\zeta\equiv L_z/N$, $0\leqslant i<N$, and $0\leqslant k\leqslant N$. The details of the discretization of Eq. (2) will be given elsewhere. We merely mention here that F is expressed as the sum of the contributions from each cell $[i\Delta x\leqslant x\leqslant(i+1)\Delta x,\ k\Delta\zeta\leqslant\zeta\leqslant(k+1)\Delta\zeta]$, in which f_{Frank} is a function of $\boldsymbol{n}_{i,k}$, $\boldsymbol{n}_{i+1,k}$, $\boldsymbol{n}_{i,k+1}$, and $\boldsymbol{n}_{i+1,k+1}$. We let the system relax from an initial condition under the fixed boundary condition at the upper surface $[\boldsymbol{n}_{i,N}=(\cos\phi,\sin\phi,0)]$, and the tangential boundary condition at the lower surface $(\boldsymbol{n}_{i,0}\cdot\boldsymbol{\nu}_i=0$, where $\boldsymbol{\nu}_i$ is the surface normal at $x=i\Delta x)$. As the initial condition, for $0°<\phi<90°$ we choose $\boldsymbol{n}_{i,k}=(\cos\phi,\sin\phi,0)$ for every i and k, and otherwise $(\phi\geqslant 90°)$ we take the equilibrium director profile of $\phi=87.5°$. We employ $\partial\boldsymbol{n}/\partial t=-(I-\boldsymbol{nn})\delta F/\delta\boldsymbol{n}$ [1] as the relaxation equation with an explicit scheme for the time evolution. Here I is a unit tensor, and the right-hand side guarantees the constraint of $\boldsymbol{n}$ being a unit vector. The time t is rescaled so that the rotational viscosity does not appear explicitly.

We choose the material parameters $K_1/K_3=0.7$, $K_2/K_3=0.5$, and $K_s/K_3=0.6$ or 1. The former two conform to the inequality $K_3>K_1>K_2$ fulfilled by most of the rodlike nematic liquid crystals [1]. $K_s/K_3=0.6$ is in agreement with the relation $K_{24}=(K_1-K_2)/2$ derived by Nehring and Saupe [15,16], and $K_s/K_3=1$ is the largest value allowed in the inequality $K_{24}\leqslant K_1$ or K_2 guaranteeing the positive definiteness of the Frank elastic energy [15,18]. As geometrical parameters, we choose $L_z=L_x$ or $L_x/2$ (see below) and $qA=\pi/160(\simeq 0.0196)$, $\pi/16(\simeq 0.196)$, $3\pi/16(\simeq 0.589)$, and 1.

Before presenting our numerical results, we recall that the anchoring energy per unit area of one-dimensional (1D) parallel grooves, derived analytically for $qA\ll 1$, reads $f_a(\phi)=(1/4)K_3q^3A^2\mathcal{F}_a(\phi)$, where [9]

$$\mathcal{F}_a(\phi)=\frac{\sin^4\phi}{g_1(\phi)}\left\{1+\frac{K_s}{K_3}\cot^2\phi\times\left(2-\frac{K_s}{K_3}\frac{g_1(\phi)g_2(\phi)-\cos^2\phi}{\sin^2\phi}\right)\right\}. \quad (3)$$

Here we have defined $g_i(\phi)=[\cos^2\phi+(K_3/K_i)\sin^2\phi]^{1/2}$ $(i=1,2)$. We note that in the derivation of Eq. (3), we have assumed infinite cell thickness $(L_z=\infty)$, which does not allow twist deformation in the bulk (however small it is, finite uniform twist in the bulk results in infinite twist elastic energy). In our numerical calculations, however, we deal with a cell of finite thickness, in which twist deformation is present in the bulk. Analytic evaluation of the total elastic energy (anchoring energy+twist energy in the bulk) along the line of Ref. [9] is highly complicated.

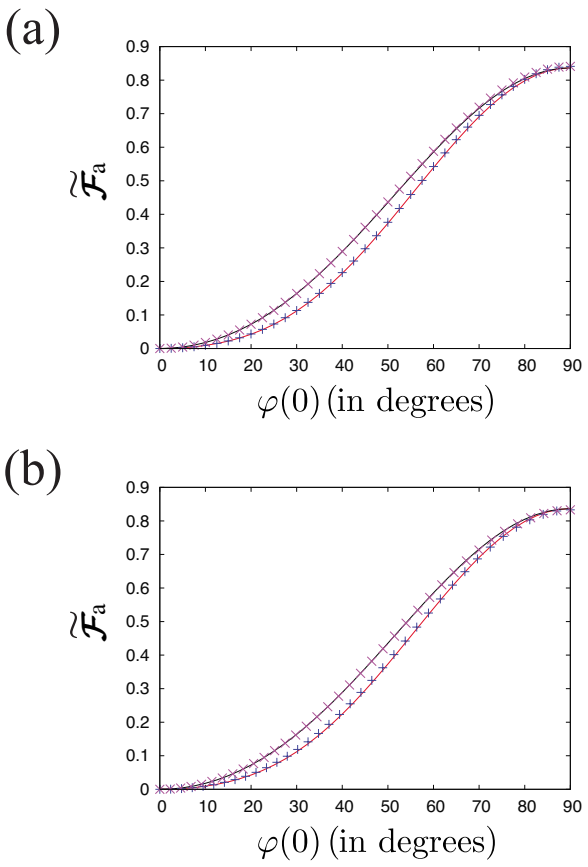

FIG. 1. (Color online) Calculated anchoring energy $\tilde{\mathcal{F}}_a$ as a function $\varphi(0)$ (in degrees) in the case of (a) $qA=\pi/160\simeq 0.0196\ll 1$ and (b) $qA=\pi/16\simeq 0.196$. The symbols $\times$ and $+$ are the results for $K_s/K_3=0.6$ and $K_s/K_3=1$, respectively. The upper and lower curves are $\mathcal{F}_a$ for $K_s/K_3=0.6$ and $K_s/K_3=1$, respectively.

To eliminate the effect of twist deformation and extract the information on the anchoring energy from the total free energy, we consider a simplified model: a nematic cell with thickness L_z sandwiched by two parallel flat surfaces; at the upper surface the director is fixed to $\boldsymbol{n}=(\cos\phi,\sin\phi,0)$, and the lower surface assumes planar alignment whose anchoring energy per unit area is written as $\tilde{f}_a(\varphi(0))$, where $\tilde{f}_a$ is now an unknown function of $\varphi(0)$. The director $\boldsymbol{n}$ in this cell then depends only on z and is written as $\boldsymbol{n}(z)=[\cos\varphi(z),\sin\varphi(z),0]$, with $\varphi(L_z)=\phi$. As the twist energy is minimized when $d\phi(z)/dz=\mathrm{const}=[\phi-\varphi(0)]/L_z$, the total free energy of the cell per unit area is given by

$$F=\tilde{f}_a(\varphi(0))+\frac{K_2}{2}\int_0^{L_z}dz\left(\frac{d\varphi}{dz}\right)^2=\tilde{f}_a(\varphi(0))+\frac{K_2[\phi-\varphi(0)]^2}{2L_z}. \quad (4)$$

For the determination of $\varphi(0)$, we calculate the azimuth of $\boldsymbol{n}$, i.e., $\varphi_{\boldsymbol{n}}\equiv\arctan(n_y/n_x)$, at all the grid points in $z\geqslant L_z/2$. A

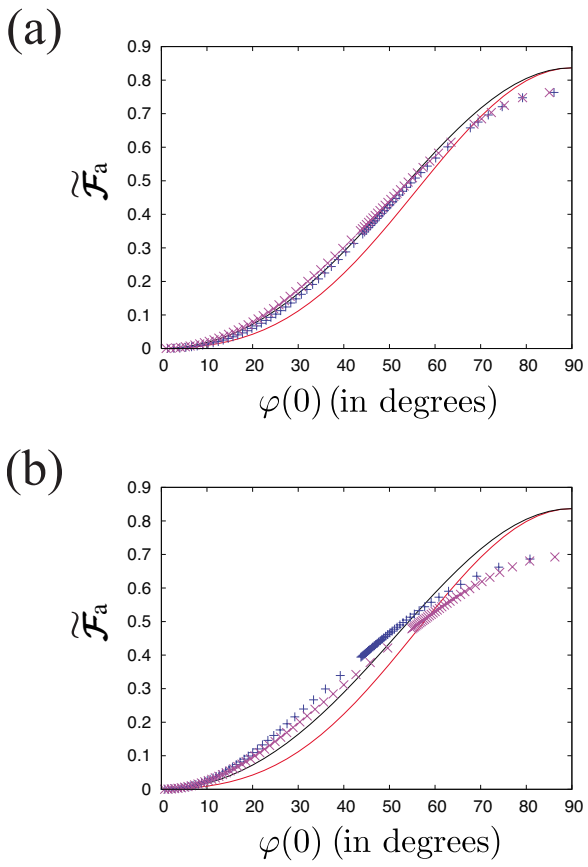

FIG. 2. (Color online) Calculated anchoring energy $\tilde{\mathcal{F}}_a$ as a function $\varphi(0)$ (in degrees) in the case of (a) $qA=3\pi/16\simeq 0.589$ and (b) $qA=1$. The symbols $\times$ and $+$ are the results for $K_s/K_3=0.6$ and $K_s/K_3=1$, respectively. The upper and lower curves are $\mathcal{F}_a$ for $K_s/K_3=0.6$ and $K_s/K_3=1$, respectively.

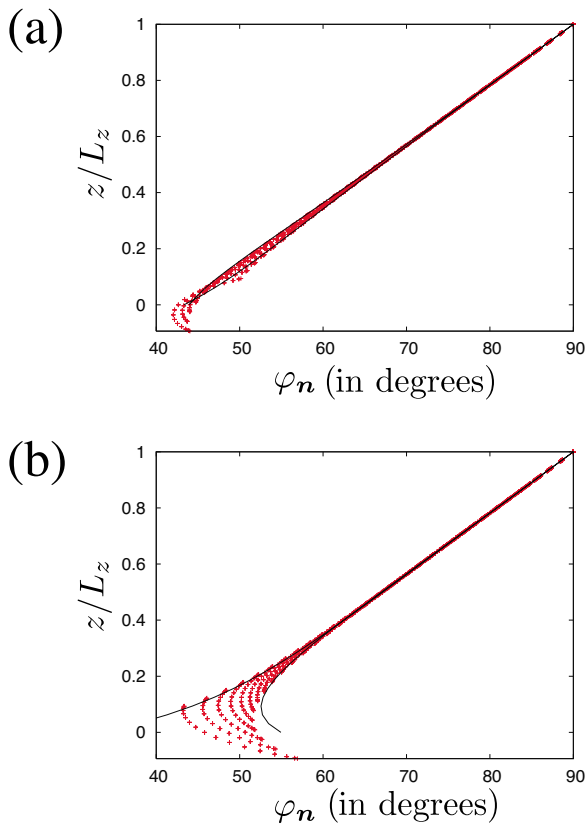

FIG. 3. (Color online) Distribution of the azimuth of the director φ_n with the variation of z/L_z in the case of $qA=3\pi/16$ and $\phi=90°$ for (a) $K_s/K_3=0.6$ and (b) $K_s/K_3=1$. Two curves in each graph specify the region in which $\varphi_n(z)$ is expected to reside in a naive theoretical argument (see text).

least-squares fit of φ_n's to $\varphi(z)=\varphi(0)+[\phi-\varphi(0)]z/L_z$ determines $\varphi(0)$. Now that $\varphi(0)$ is known and F has been calculated numerically, the "numerical" anchoring energy $\tilde{f}_a$ can be determined as a function of $\varphi(0)$ from Eq. (4). We introduce a rescaled numerical anchoring energy $\tilde{\mathcal{F}}_a=\tilde{f}_a/(\frac{1}{4}K_3q^3A^2)$, which can be directly compared with a rescaled analytic anchoring energy $\mathcal{F}_a$ in Eq. (3). We notice here that $\mathcal{F}_a$ is independent of qA, and therefore in the following figures one will find the same functional form of $\mathcal{F}_a$ as a function of $\varphi(0)$.

In Fig. 1, we plot the rescaled numerical anchoring energy $\tilde{\mathcal{F}}_a$ as a function of the azimuthal angle $\varphi(0)$ for $qA=\pi/160$ and $\pi/16$, respectively. In these calculations we have chosen $L_z=L_x$. We find an excellent agreement of $\tilde{\mathcal{F}}_a$ with the anchoring energy $\mathcal{F}_a$ calculated analytically for $qA\ll 1$, which manifests the validity of our numerical treatments and of our analytical formula, Eq. (3). Note the remarkable agreement in Fig. 1(b), or in the case of $qA=\pi/16\simeq 0.2$, for which $qA\ll 1$ cannot be postulated. We also notice that in the case of $qA=\pi/160$, twist deformation in the bulk is almost negligible and $\varphi(0)$ and $\phi[=\varphi(L_z)]$ are almost equal. It is therefore natural that the total free energy F is almost equal to the (dimensional) anchoring energy $\frac{1}{4}K_3q^3A^2\tilde{\mathcal{F}}_a$. On the other hand, for $qA=\pi/16$, twist deformation is indeed present and the total free energy F, without the subtraction of the twist contribution, does not agree with analytical anchoring energy $\frac{1}{4}K_3q^3A^2\mathcal{F}_a$.

Before examining further results for $qA=3\pi/16$ and 1 in Fig. 2, we notice that in the previous cases in Fig. 1 twist deformation is absent when $\phi=90°$, or in other words $\varphi(0)=90°$ because anchoring torque of those surfaces with $qA=\pi/160$ or $\pi/16$ is small enough. The data presented there are results for $0\leqslant\phi\leqslant 90°$. On the other hand, for $qA=3\pi/16$ and 1, $\varphi(0)$ is smaller than 90° when $\phi=90°$ due to larger anchoring torque. Therefore the data in Fig. 2 contain results for "overtwisted" configurations with $\phi>90°$. We also note that we have chosen $L_z=L_x/2$ for $qA=1$, although $L_z=L_x$ has been used for $qA=3\pi/16$ as in the previous cases. This is because with this choice reliable results can be extracted for a larger range of $\varphi(0)$. We have observed that for $\varphi(0)\lesssim 40°$, the choices $L_z=L_x/2$ and $L_z=L_x$ yield the same dependence of $\tilde{\mathcal{F}}_a$ on $\varphi(0)$.

Now let us investigate the results in Fig. 2 for $qA=3\pi/16$ and 1. It is not surprising that the numerical results deviate from analytical anchoring energy derived for $qA\ll 1$. Nevertheless, the deviations are not large, in particular in the case of $qA=3\pi/16$ and $K_s/K_3=0.6$. Therefore we can say from our results that the anchoring energies deter-

mined numerically give a semiquantitative agreement with analytical ones even when $qA \ll 1$ does not hold.

The quantitative agreement between analytical and numerical anchoring energy, in particular when $qA=3\pi/16$ and $K_s/K_3=0.6$, is somewhat surprising. To find out the reason for this agreement, we show in Fig. 3 the azimuth of the director $\varphi_n \equiv \arctan(n_y/n_x)$ as a function of z/L_z at all the grid points in our numerical system with $qA=3\pi/16$, $\phi=90°$, and $K_s/K_3=0.6$ or 1. We find that in the bulk (not in the vicinity of the lower surface) almost uniform twist is present as has been argued above. We also show in Fig. 3 the range of φ_n expected by a naive theoretical argument: φ_n should be the superposition of uniform twist $(\varphi_{tw}(z) \equiv \varphi(0)+[\phi-\varphi(0)]z/L_z)$ and azimuthal distortions induced by the grooved surface, and therefore is expected to be in between $\varphi_{tw}(z) \pm \arcsin\{n_y^{max}[\varphi(0),z]\}$. Here $n_y^{max}(\varphi,z)$ is the maximum azimuthal distortion calculated in our previous analytical argument, which is [9]

$$n_y^{max}(\varphi,z) = qA \sin\varphi(\cos\varphi \exp[-qzg_1(\varphi)]/g_1(\varphi) + (K_s/K_3)\cot^2(\varphi)\{\cos\varphi \exp[-qzg_1(\varphi)]/g_1(\varphi) - g_2(\varphi)\exp[-qzg_2(\varphi)]/\cos\varphi\}).$$

Figure 3 clearly indicates that the azimuthal angle profile $\{\varphi_n\}$ falls onto the region expected by the above naive theoretical argument. This implies that the difference between the director profiles of numerical calculation and analytical argument is small, resulting in a relatively good agreement between the numerical and the analytical anchoring energies. We also find from Fig. 3 that deviation of the azimuthal angle profile from that of a uniform twist is smaller when $K_s/K=0.6$. This might be the reason why $K_s/K=0.6$ yields a better agreement between the numerical and the analytical anchoring energies.

In conclusion, to elucidate the anchoring properties of a surface with 1D parallel grooves, we have performed numerical calculations of the energy of a nematic cell made up of such a grooved surface and a flat surface. When $qA \lesssim 0.2$, with q and A being the wave number and height of the grooves, the anchoring energy calculated numerically is in excellent agreement with theory, indicating the applicability of our theory of surface anchoring in that range of qA. For $qA \simeq 0.6$ and 1, we also find a semiquantitative agreement of the numerical anchoring energy with the analytical one. Considering the assumption of $qA \ll 1$ in deriving the analytical anchoring energy, our findings are somewhat surprising in that the analytical anchoring energy can describe the quantitative as well as qualitative feature of the anchoring of grooved surfaces even when $qA \ll 1$ does not hold. We finally notice that a similar calculation can be done also for two-dimensionally patterned surfaces, which will be presented in a future work.

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