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Nonlinear theory of dislocations in smectic crystals: An exact solution

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It is shown that the strain field of an edge dislocation in a smectic crystal must be described in the framework of nonlinear theory, even far away from the core region. We present an exact solution of this nonlinear problem. The result of the linear theory is recovered in the limit of large bending rigidity. [S1063-651X(99)50605-3]

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The strain field of point and linear defects in crystals decays with the distance from the defect, so that the long range distortion around the defects can be described within the framework of the linear theory of elasticity. The same approach has been used by de Gennes to describe edge dislocations in a smectic crystal [1]. This linear theory is believed to be exact far from the dislocation core, and it is presented in text books on physics of liquid crystals and also in the more general context of the theory of elasticity (see, for example, [2,3]). The intrinsic anisotropy of smectics, however, means that nonlinear effects can be important even for small strains, and the Helfrich instability [4], the corrugation of smectic layers in a stretched smectic film, is a well-known example.

In this Rapid Communication we show that the linear theory of edge dislocations in smectics [1] is valid only in the limit $b \ll \lambda$, where *b* is the Burgers vector and λ is the length scale in the elastic energy functional. In the general case where $b \sim \lambda$ nonlinearities must be taken into account to describe the asymptotic behavior even at large distances from the core. To the best of our knowledge this is the first instance where the asymptotic distortion field induced by the defect in a three-dimensional object must be treated by non-linear theory. Moreover, we give an exact solution of the nonlinear equation for the displacement field around a dislocation.

For small strains the distortion energy of a smectic is [2]

$$F = \frac{1}{2} \int dx dz \{ A [\partial_z u - \frac{1}{2} (\partial_x u)^2]^2 + B (\partial_x^2 u)^2 \}.$$
(1)

Here u(x,z) is the smectic displacement field, *A* is the elastic modulus, and *B* is the bending modulus; the dislocation lies along the *y* axis. The intrinsic length scale λ is given by $\lambda = (B/A)^{1/2}$. In linear approximation the strain field for the edge dislocation is obtained [1] (see also [2]) as

$$\partial_z u = -\frac{bx}{8(\pi\lambda)^{1/2} z^{3/2}} \exp\left[-\frac{x^2}{4\lambda z}\right]$$
(2)

and

$$\partial_x u = \frac{b}{4(\pi\lambda z)^{1/2}} \exp\left[-\frac{x^2}{4\lambda z}\right]$$
(3)

for z > 0. The most significant change of the displacement field occurs in the region $x \sim \sqrt{\lambda z}$. The linear approximation is valid for $(\partial_x u)^2 / |\partial_z u| \ll 1$. However, this ratio is of order b/λ and independent of z in the important region. Thus, a nonlinear theory must be applied to describe the general case $b \sim \lambda$.

The full nonlinear equation is obtained by variation of the energy, Eq. (1), and reads

$$\lambda^2 \partial_x^4 u - \partial_z^2 u + 2(\partial_x u) \partial_z \partial_x u + (\partial_x^2 u) \partial_z u - \frac{3}{2} (\partial_x u)^2 \partial_x^2 u = 0.$$
(4)

Let us measure all the lengths (u,x,z,b) in units of λ . If we assume that, as in the linear approximation, the displacement field u(x,z) depends only on the variable $v = x/\sqrt{z}$ the problem reduces to the solution of a third order ordinary differential equation for the strain field $\phi = du/dv = u'$:

$$\phi''' = \frac{v^2}{4}\phi' + \frac{3v}{4}\phi + \phi^2 + \frac{3v}{2}\phi\phi' + \frac{3}{2}\phi^2\phi' \qquad (5)$$

subject to the constraint

$$u(+\infty) - u(-\infty) = \int_{-\infty}^{\infty} \phi dv = b/2.$$
 (6)

Fortunately an exact solution of Eq. (5) exists that meets all physical requirements. Indeed, it is easily checked that under the condition

$$\phi' = -\frac{1}{2}(\phi^2 + v\phi),$$
 (7)

Eq. (5) is automatically satisfied. The general solution of Eq. (7) is

$$\phi = \frac{2e^{-v^2/4}}{\int_{-\infty}^{v} e^{-t^2/4} dt + C}$$
(8)

where *C* is a constant of integration to be determined by Eq. (6). Finally, in the original, dimensioned variables the displacement field u is given by

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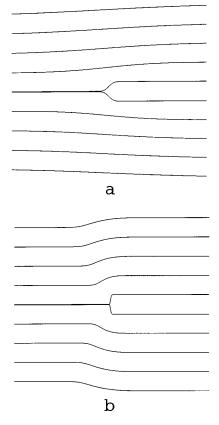


FIG. 1. The distortions induced by a dislocation in a smectic crystal: (a) $\lambda = 2b$; (b) $\lambda = 0.05b$.

$$u = 2\lambda \ln \left[1 + \frac{e^{b/4\lambda} - 1}{2\sqrt{\pi}} \int_{-\infty}^{x/\sqrt{\lambda z}} e^{-t^2/4} dt \right].$$
(9)

In the limit $b \ll \lambda$ the result of the linear theory [1] is recovered,

$$u \approx \frac{b}{4\sqrt{\pi}} \int_{-\infty}^{x/\sqrt{\lambda z}} e^{-t^2/4} dt.$$
 (10)

We note that the field ϕ is an even function of v in the linear theory, whereas nonlinear effects destroy this symmetry. Figure 1 presents the distortion field induced by a dislocation which we plot according to the exact result, Eq. (9). Figure 1(a) corresponds to the small ratio $b/4\lambda = 1/8$ and the result of linear theory, Eq. (10), is a good approximation. The displacement field changes mainly in the range of positive and negative x, $|x| \sim \sqrt{\lambda z}$. Figure 1(b) corresponds to the

strongly nonlinear case, $b/4\lambda = 5$. In this case the asymmetry becomes very pronounced: the displacement field changes mainly in the range of negative *x* and $|x| \sim \sqrt{bz} > \sqrt{\lambda z}$ (linear theory still predicts symmetric range $|x| \sim \sqrt{\lambda z}$).

Normally λ is several times larger than the interlayer distance. Together with the fact that the actual expansion parameter is $b/4\lambda$ this makes the linear theory a good approximation in many experimental situations. However, for a finite density of dislocations in some localized region the effective Burgers vector can be large enough to make the nonlinear effects observable.

We now discuss another structure that appears as a limiting case of our exact solution. Equation (8) gives for C=0 the displacement field

$$u = 2\lambda \ln \left[\frac{1}{2\sqrt{\pi}} \int_{-\infty}^{x/\sqrt{\lambda z}} e^{-t^2/4} dt \right]$$
(11)

[where we have chosen $u(+\infty)=0$] that describes the following texture. For $x \ge \sqrt{\lambda z}$ there are almost flat smectic layers and for negative $x(|x| \ge \sqrt{\lambda z})$ the displacement field, $u = -x^2/2z$, corresponds to parabolic layers where z is the radius of curvature. This parabolic structure is the beginning of a circular structure. The smooth matching between the structures with zero and finite curvatures is in the region $|x| \sim \sqrt{\lambda z}$.

To conclude, we have found that even for a small strain, $\partial_z u \ll 1$ and $\partial_x u \ll 1$, the asymptotic distortion field around the edge dislocation in smectics *must* be treated in the framework of nonlinear theory using the elastic energy functional, Eq. (1). We have found an exact solution of this problem where the displacement field depends only on a scaling variable. Dislocations in smectics lie somewhere in between point defects, which can still be treated by linear theory, and cases with a localized force or linear distribution of forces. The angle $\partial_x u$ is of order unity in the latter, requiring the use of a fully nonlinear theory beyond the functional in Eq. (1). Such work is in progress.

Our findings should also be applicable to those systems which have common features with smectics such as block copolymer films, charge density waves, spin density waves, the vortex lattices in superconductors, and in superfluid ³He and ⁴He.

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