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Grain boundary structure in incommensurate smectics: a signature of phasons

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Abstract. We consider a tilt grain-boundary with small angle θ in an incommensurate smectic A_{ic} liquid crystal with ordering wavenumbers q_1, q_2 and sample thickness h in the direction normal to the layers. For $q_i\theta h \ll 1$, a limit well within the reach of experiment, we find that the dislocation array which forms such a boundary has a spacing $D \sim h^{1/5}\theta^{-4/5}$. This prediction, which is qualitatively different from that obtained for periodic smectics by Nallet and Prost, should serve as a decisive test for the existence of phasons and hence for the truly incommensurate nature of these systems.

Although the incommensurate smectic A phase (hereafter referred to as the A_{ic}) was discovered by Ratna *et al* [1] in 1985, there have been, so far as we know, no experimental studies of its mechanical properties or low-energy excitations. We show here that an important signature of the quasiperiodic nature of this phase, a direct result of the existence [2] of an additional (phason) broken-symmetry mode, should be seen in the structure of small-angle grain-boundaries. This is a brief summary of the work; details can be found in [3].

The A_{ic} is a three-dimensional system whose time-averaged density field has two static, one-dimensional modulations in the z direction, with wavenumbers q_1 and q_2, where q_1/q_2 is irrational. More precisely, in the experiment of Ratna *et al* [1], the ratio varies continuously from 1 to 2 as a function of temperature, and is hence *generically* irrational. Writing the density field for the system as

$$\rho(r) = \rho_0 + A_1 e^{iq_1(z-u_1)} + A_2 e^{iq_2(z-u_2)} + \text{cc} + \text{higher orders} \qquad (1)$$

this means that spatially uniform changes in the individual layer displacement fields u_1 and u_2, independently, cost no free-energy. However, the physics of distortions in which one set of layers moves relative to another ($u_1 \neq u_2$) is quite different from that in which the two move jointly ($u_1 = u_2$). It is evident, in particular, that joint rigid rotations of the two density waves ($\partial_x u_1 = \partial_x u_2 = \text{constant}$) should cost no energy while relative rotations ($\partial_x u_1 \neq \partial_x u_2$), even when spatially uniform, should carry a bulk energy cost [2]. Defining [2] the joint, or phonon (u), and relative, or phason (w) displacement fields $u = \alpha[su_1 + (1-s)u_2]$ and $w = \alpha^{-1}(u_1 - u_2)$, for arbitrary real α and $0 < s < 1$, it can be shown that the elastic free-energy for the A_{ic} is the sum of a normal smectic elastic

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energy for the u-field and an 'xy'-like square-gradient energy (with a trivial anisotropy) for the w field:

$$H = \frac{1}{2}\int [B(\partial_z u)^2 + K(\nabla_\perp^2 u)^2 + B_w(\partial_z w)^2 + C_w(\nabla_\perp w)^2]\, \mathrm{d}^3x. \tag{2}$$

Fundamental dislocations in the A_{ic} can be made [2] by introducing a single extra half-layer in one or other of the two density waves. Compound dislocations can be made by combining these fundamental dislocations. A general dislocation in the A_{ic} is thus characterized by a two-component vector $(b_1, b_2) = (m_1 d_1, m_2 d_2)$, where d_1 and d_2 are the incommensurate periods, and m_1, m_2 (integers) are the numbers of extra half-layers inserted into density-waves 1 and 2. In terms of the u and w variables, we can define $b_u = \alpha[sb_1 + (1-s)b_2]$ and $b_w = \alpha^{-1}(b_1 - b_2)$. The fundamental irrationality of $\zeta = d_1/d_2$ guarantees that b_w is never zero: in fact one can show [3] that for a generic irrational ζ, the smallest b_w for a given b_u is

$$b_w^{\min} \propto d_1^2/b_u. \tag{3}$$

Since b_w is never zero, and since the energy-cost of w distortions is square-gradient, the interaction between a pair of straight edge dislocations in the A_{ic} is utterly different [2] from that in a periodic smectic: the dominant interaction at large distances R in any direction is essentially proportional to $A_w b_w^2 \ln(R/a)$ where A_w is an effective w elastic constant and a is a microscopic length of order of the layer spacing. Let us now see how these unique characteristics lead to the predictions made above, by constructing a dislocation model for a tilt grain-boundary with small-angle θ in the A_{ic}.

As a first candidate for such a model, consider an array of identical, straight edge dislocation lines with Burgers vector (b_u, b_w) and spacing $D = b_u/\theta$, lying parallel to the y axis in the x–y plane and dividing the sample into an upper and a lower grain. The usual description [4] of grain boundaries as dislocation arrays gives a rotation through an angle θ of one grain with respect to the other, i.e. $|\partial u/\partial x| \to \infty$ as $|z| \to \infty$. But the same argument applied to the w part of the Burgers vector implies that $|\partial w/\partial x| \to \infty$ as $|z| \to \infty$, so that both grains suffer costly bulk w rotations. The array as constructed is not a grain boundary.

The way out of this [5] is to build an array of length L of dislocations with mean spacing D, with total $b_u \propto L$ and with the individual b_w values roughly equal in magnitude but alternating quasiperiodically in sign in such a way that the total $b_w \to 0$ as the size $L \to \infty$. As a result of equation (3), the best one can do is $b_w \propto L^{-1}$, which is sufficient. There is still an infinite number of ways of doing this, since only $b_u/D = \theta$ is fixed. We must find the grain boundary with the lowest energy for a given θ. In crystals, this requires dislocations with the smallest possible Burgers vector. In periodic smectics [6], as a result of the unusual nature of the core energy [7], the dislocations in a grain boundary can lower the energy by clumping. We shall see next that this happens in the A_{ic} as well, but that this is due, for $q_i \theta h \ll 1$, to phasons. In this limit, the effects of [7] are negligible.

To calculate the energy of a grain boundary in the A_{ic} note first that since the dislocations are lying side-by-side, i.e. at the same z coordinate, the nature of the u elastic energy of a smectic ensures [8] that there is no contribution to their interaction energy from the u field. For $q_i h\theta \ll 1$, there are only two relevant pieces in the grain-boundary energy. We discuss each in turn.

First, adjacent dislocations have, in general opposite b_w, and hence attract. The contribution of more distant dislocations is screened, so that a good estimate of this

contribution per unit area of grain boundary, E_{phason}, is obtained by taking the typical w interaction energy per nearest neighbour pair, per unit length of dislocation line, and dividing by the spacing D. This gives

$$E_{\text{phason}} \propto B_w(b_w^2/D)\ln(h/a) \tag{4a}$$

which, putting in as small a b_w as possible, from (3), and using the fact that $b_u/D = \theta$, becomes

$$E_{\text{phason}} \propto B_w\theta(a^4/b_u^3)\ln(hb_u/a^2). \tag{4b}$$

Here B_w is a typical w elastic constant and a is a microscopic length of the order of the layer spacing. Note here that the logarithm is cut off by the sample thickness h rather than the spacing D as a result of the condition $q_i\theta h \ll 1$. Note also that (4*b*) favours large b_u as a means of getting rid of unwanted energy stored in the w field.

The other contribution to the energy per unit area is the 'wedge energy' [6], which arises because, in a thin sample, the parabolic regions of appreciable u-strain above and below each edge dislocation do not overlap, so that between dislocations, the layers are splayed apart. This local departure of the layer spacing from its preferred value costs an energy per unit area [6]

$$E_{\text{wedge}} = Bb_u^2/12h. \tag{5}$$

This term competes with (4*b*) by favouring small b_u. Treating b_u as a continuous variable (which can be justified [3]) and minimizing the total energy per unit area (4*b*) + (5), we find the optimal values b^* and D^* for b_u and D:

$$b^* = g(\theta h/a)^{1/5}/a = \theta D^* \tag{6}$$

where the coefficient g varies roughly as $(\ln b^*)^{1/5}$ and can therefore be treated essentially as a constant. It is straightforward to show [3] that the result is consistent with $q_i\theta h \ll 1$.

The condition $q_i\theta h \ll 1$ means that our results should show up only in the limit of very small angles, at least for thermotropic systems, which are the only ones where the A_{ic} has been found. For such systems, in the classical wedge geometry [9] used to produce a grain boundary in smectics, assuming q_i is of order 3×10^{-7} cm and a thickness $h =$ 0.1 mm, θ should be about 0.05°. We are told [10] that this, or an equivalent set-up in the geometry of [6] is feasible. A positive result in such an experiment would be the first confirmation of the existence of phasons in the A_{ic}. A negative result would cast doubt on the incommensurate nature of the phase.

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