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Point defects and lock-in faults in columnar phases

J. Prost[a]
[a] Laboratoire de Physico-Chimie Théorique, URA 1382 du CNRS, Ecole Supérieure de Physique et de Chimie Industrielles de la Ville de Paris, Paris Cedex 05, France

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Point defects and lock-in faults in columnar phases

by J. PROST

Laboratoire de Physico-Chimie Théorique, URA 1382 du CNRS, Ecole Supérieure de Physique et de Chimie Industrielles de la Ville de Paris, 10, rue Vauquelin, F-75231 Paris Cedex 05, France

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We show the existence of point defects connected by strings in columnar phases. The most interesting consequence is the increase, by several orders of magnitudes, of the bend elastic modulus as compared to values for nematics.

1. Introduction

Dislocations in columnar phases have already been discussed [1–3]. Screw dislocations are particularly original since they do not involve any column discontinuity [1, 2]. A pair of them of opposite directions and the same Burgers' vector, distant from a lattice spacing, as shown in figure 1 (*a*), constitutes a linear defect, topologically stable, which we shall call a lock-in fault line. The corresponding structure is unperturbed, except in a plane where the columns jump from one lock-in site to the next (or more generally to an equivalent one). These lines can end on point defects, which are column extremities (see figure 1 (*b*)). This situation is fairly similar to that of Dirac's monopoles [4]. The point defect of order two in figure 2 is topologically stable, in contrast to that shown in figure 1 (*c*). Any dislocation configuration can be represented as an ensemble of column extremities and lock-in fault lines, and vice versa. In this paper, we calculate the deformation field corresponding to an infinite and semi-infinite lock-in fault line, and discuss the macroscopic behaviour of columnar phases in the presence of densities of such defects.

2. Strain field of a lock-in fault line

The strain can be described by two vectors in a columnar phase: $\mathbf{m}^x$ and $\mathbf{m}^y$ represent local compressions and rotations of the lattice: m_x^x (m_y^y) compression along $x(y)$, m_z^x (m_z^y) the rotation around a $y(x)$ axis, $\frac{1}{2}(m_y^x - m_x^y)$ the lattice rotation around the z axis. In the absence of dislocations $\mathbf{m}^x = \nabla u_x$, $\mathbf{m}^y = \nabla u_y$ and u_x, u_y are the column displacements. The dislocations obey similar laws as in crystals [5, 6]

$$\mathbf{Curl}\,\mathbf{m}^\alpha = \mathbf{J}^\alpha, \tag{1}$$

in which $\mathbf{J}^\alpha$ is a vector current oriented along the line, with a modulus equal to that of the dislocation Burgers' vector. Current lines obey the conservation rule

$$\mathrm{Div}\,\mathbf{J}^\alpha = 0. \tag{2}$$

As a consequence, the strain field surrounding a lock-in fault line of infinite extent along Ox, is described by

$$\left.\begin{aligned} \mathbf{Curl}\,\mathbf{m}^x &= a^2 \frac{\partial \delta_y}{\partial y}\,\delta_z \hat{x}, \\ \mathbf{Curl}\,\mathbf{m}^y &= 0. \end{aligned}\right\} \tag{3}$$

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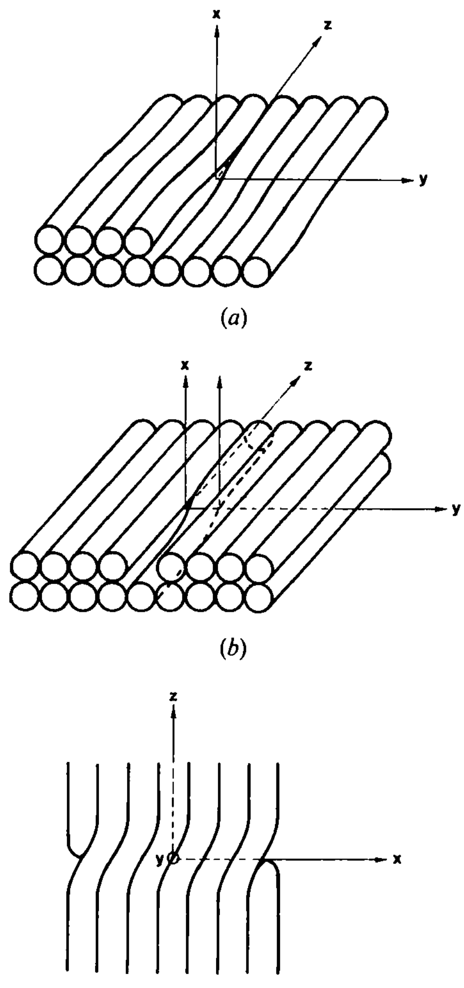

Figure 1. (*a*) A screw dislocation in a columnar phase, using a square lattice for simplicity. (*b*) A lock-in fault line in the same lattice; the two axes parallel to the x axis determine the screw dislocation dipole aspect of this line. (*c*) A lock-in fault line in the xz plane. This line ends on a right column extremity (positive on the left side, negative on the right; the signs are defined with respect to z).

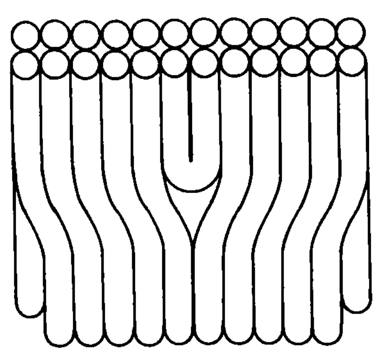

Figure 2. A topologically stable point defect of charge $+2$.

This expression corresponds to a square lattice, more generally we should replace a^2 by S the area occupied by a column ($a^2\sqrt{3}$ for a triangular lattice).

Mechanical equilibrium requires

$$\left.\begin{aligned} 0 &= B\frac{\partial}{\partial x}(m_x^x + m_y^y) + C\frac{\partial}{\partial x}(m_x^x - m_y^y) + C\frac{\partial}{\partial y}(m_y^x + m_x^y) - k_3\frac{\partial^3}{\partial z^3}m_z^x, \\ 0 &= B\frac{\partial}{\partial y}(m_x^x + m_y^y) + C\frac{\partial}{\partial y}(m_y^y - m_x^x) + C\frac{\partial}{\partial x}(m_y^x + m_x^y) - k_3\frac{\partial^3}{\partial z^3}m_z^y, \end{aligned}\right\} \tag{4}$$

which corresponds to the elastic energy [7]

$$F = \tfrac{1}{2}\int dv\left\{B(m_x^x + m_y^y)^2 + C\left((m_x^x - m_y^y)^2 + (m_y^x + m_x^y)^2\right) + k_3\left(\left(\frac{\partial}{\partial z}m_z^x\right)^2 + \left(\frac{\partial}{\partial z}m_z^y\right)^2\right)\right\}. \tag{5}$$

The solution in Fourier space ($\tilde{\lambda}_3^2 = k_3/C$) is

$$\left.\begin{aligned} m_x^x &= m_y^y = m_x^y = m_z^y = 0, \\ m_y^x &= \frac{-a^2\tilde{\lambda}_3^2 q_z^3 q_y}{q_y^2 + \tilde{\lambda}_3^2 q_z^4}, \qquad m_z^x = \frac{a^2 q_y^2}{q_y^2 + \tilde{\lambda}_3^2 q_z^4}, \end{aligned}\right\} \tag{6}$$

or in real space

$$\left.\begin{aligned} m_y^x &= \frac{a_z^2}{8(\pi\tilde{\lambda}_3)^{1/2}}\frac{\partial}{\partial y}\left(|y|^{-3/2}\exp(-z^2/4\tilde{\lambda}_3|y|)\right), \\ m_z^x &= \frac{\pm a^2}{4(\pi\tilde{\lambda}_3)^{1/2}}\frac{\partial}{\partial y}\left(|y|^{-1/2}\exp(-z^2/4\tilde{\lambda}_3|y|)\right). \end{aligned}\right\} \tag{7}$$

This expression is a derivative of that corresponding to the strain field of a screw dislocation, as expected.

The line tension is

$$\gamma = \frac{k_3 a^4}{2}\int\frac{d^2q}{(2\pi)^2}\frac{q_z^2 q_y^2}{q_y^2 + \tilde{\lambda}_3^2 q_z^4} \tag{8}$$

and the integral depends on the ultraviolet cut-off Λ. A consistent choice is

$$\Lambda_y \propto a^{-1}, \qquad \Lambda_z \propto a^{-1/2}\tilde{\lambda}_3^{-1/2} \tag{9}$$

which leads to

$$\gamma \propto Ca^{3/2}\tilde{\lambda}_3^{1/2}. \tag{10}$$

We still have to add the core energy: we can easily become convinced that the characteristic length of the lock-in fault is precisely Λ_z. Indeed, the lock-in energy is

$$F_b = \int\left\{a^2\frac{k_3}{2}\left(\frac{\partial^2 U^x}{\partial z^2}\right)^2 - a^2\bar{B}\cos\left(\frac{2\pi u}{a}\right)\right\}dz, \tag{11}$$

that is a Euler–Lagrange equation

$$\frac{\partial^4\phi}{\partial z^4} + 4\pi^2\lambda_3^{-2}a^{-2}\sin\phi = 0, \tag{12}$$

with $\phi = (2\pi u)/a$, and a characteristic length $(\lambda_3 a/2\pi)^{1/2}$, hence an energy scaling like equation (10).

Thus

$$\gamma = \eta C a^{3/2} \lambda_3^{-1/2} \tag{13}$$

in which η is a numerical coefficient. This result is similar to that obtained with screw dislocations. It corresponds to a line perpendicular to the column axis. It is possible that tilted lines have a lower energy, but the following considerations should not be significantly modified if this is the case. γ is an elastic energy; the corresponding free energy is

$$f = \gamma - \frac{k_B T}{a} \eta', \tag{14}$$

in which η' is another number of order unity. There is *a priori* no guarantee that f be positive. In fact upon approaching the melting transition γ decreases whereas the entropic term increases. Thus f becomes negative before the mean field transition. The same remark holds for dislocations, but it seems reasonable to assume that the line energy of lock-in faults is smaller than that of dislocations. As a result it vanishes at lower temperatures, and it seems legitimate to study the influence of densities of such lines on the macroscopic behaviour of columnar phases. We discuss this matter in §4.

3. A semi-infinite line

We consider a line extending along the positive side of the $\hat{x}$ axis. The source term reads now (still considering a square lattice for the sake of simplicity)

$$\left.\begin{aligned} \mathbf{Curl}\,\mathbf{m}^x &= a^2 \frac{\partial}{\partial y} \delta_y \delta_z Y_x - a^2 \delta_y \delta_z \delta_x \hat{y}, \\ \mathbf{Curl}\,\mathbf{m}^y &= 0; \end{aligned}\right\} \tag{15}$$

Y_x is the unit step function. The source term along $\hat{y}$, deserves particular attention. On the one hand it is written in such a way that the dislocation line circuit is conservative; it is an edge dislocation segment of unit length. On the other hand, it does correspond to a column extremity. Indeed, from equation (15) we easily find

$$\frac{\partial}{\partial x} m_z^x + \frac{\partial}{\partial y} m_z^y - \frac{\partial}{\partial z}(m_x^x + m_y^y) = a^2 \delta_x \delta_y \delta_z, \tag{16}$$

or, introducing $\mathbf{n}$ the unit vector along the column axis

$$\mathrm{Div}\left(\frac{\mathbf{n}}{a^2}\right) = \delta_x \delta_y \delta_z. \tag{17}$$

In this equation the meaning of the column extremity is clear. The sign, i.e. column beginning or ending, depends on the choice of $\mathbf{n}$.

The generalization gives

$$\mathrm{Div}\left(\frac{\mathbf{n}}{a^2}\right) = \rho(\mathbf{r}), \tag{18}$$

where $\rho(r)$ is the algebraic density of column extremities. As already pointed out in (1), the splay deformation is directly related to $\rho(\mathbf{r})$.

The strain field corresponding to equation (15), can again be calculated in Fourier space. We find that the lattice dilation $\theta = m_x^x + m_y^y$ depends only on the point source

$$\left.\begin{aligned} \theta(q) &= \frac{ia^2\lambda_3^2 q_z^3}{q_\perp^2 + \lambda_3^2 q_z^4} \\ \text{with} \qquad \lambda_3^2 &= k_3/(B + C) \end{aligned}\right\} \tag{19}$$

or in real space

$$\theta = \lambda_3^2 a^2 \frac{\partial^3}{\partial z^3} G(x_\perp, z), \tag{20}$$

with

$$G(x_\perp, z) = \frac{1}{16\pi\lambda_3}\frac{z}{x_\perp} K_{1/4}(z^2/2\lambda_3 x_\perp)[I_{1/4}(z^2/2\lambda_3 x_\perp) + I_{-1/4}(z^2/2\lambda_3 x_\perp)], \tag{21}$$

$x_\perp = \sqrt{(x^2 + y^2)}$, $K_{1/4}$ and $I_{\pm 1/4}$ are modified Bessel functions [8]. Similarly, the longitudinal part of the column tilt, $\delta\mathbf{n}_\perp = m_z^x\hat{x} + m_z^y\hat{y}$ depends again only on the point source

$$\delta n_\perp(q) = \frac{-ia^2\mathbf{q}_\perp}{q_\perp^2 + \lambda_3^2 q_z^4}, \tag{22}$$

or

$$\delta\mathbf{n}_\perp(x_\perp, z) = -a^2\nabla_\perp G(x_\perp, z). \tag{23}$$

For $z^2 \gg \lambda_3 x_\perp$, $G \sim 1/z$ and the dilation decreases like $1/z^4$, whereas the columns are not tilted. For $z^2 \ll \lambda_3 x_\perp$, $G \sim 1/(\lambda_3 x_\perp)^{1/2}$; the lattice dilation is negligible whereas the tilt decreases like $x_\perp^{-3/2}$. Sufficiently far from the extremity the strain of the infinite line is of course recovered.

These dependences show that the direct interaction energy between two extremities (one being at the origin, the other at the point $x_\perp, z$) decreases like z^{-3}, if $z^2 \gg 2\lambda_3 x_\perp$, and like $x_\perp^{-1/2}$, if $z^2 \ll 2\lambda_3 x_\perp$. These are long range interactions. For two extremities belonging to the same line, the dominant interaction is, however, that due to the line tension, since it corresponds to a force independent of distance.

4. Lock-in fault line densities

This is a particular case of dislocation loop densities, for which a magnetic analogy is useful [6, 9]. However, we can easily be convinced that only the tube extremities experience a Peach–Kohler force, in a homogeneous stress (a force linked to stress gradients does exist on the lines but it does not lead to a renormalization of the elastic moduli). Under those conditions, an electrostatic analogy is simpler. The force exerted on the charges is

$$F_z = \varepsilon a^2(\sigma_{xx} + \sigma_{yy}); \qquad F_\alpha = -\varepsilon a^2 \sigma_{\alpha z}; \qquad \alpha \in (x, y). \tag{24}$$

The vector

$$\boldsymbol{\sigma} = \begin{bmatrix} \sigma_{xz} \\ \sigma_{yz} \\ \sigma_{xx} + \sigma_{yy} \end{bmatrix}$$

is the analogue of the electric field; $\epsilon = +1$ (resp. -1) corresponds to a column beginning (resp. ending). The analogy with electrostatics allows us to write

$$\left.\begin{aligned} \sigma_{xx} &= B(m_x^x + m_y^y - p_z) + C(m_x^x - m_y^y), \\ \sigma_{yy} &= B(m_x^x + m_y^y - p_z) + C(m_y^y - m_x^x), \\ \sigma_{\alpha z} &= -K_3 \frac{\partial^2}{\partial z^2}(m_z^\alpha - p_\alpha). \end{aligned}\right\} \tag{25}$$

The other components of the stress tensor are not modified. As in electrostatics, p is the first moment of the charge distribution

$$\mathbf{p} = \frac{a^2}{v}\int_v \mathbf{r}\,\rho(r)\,dv. \tag{26}$$

In thermal equilibrium, $p_\alpha = 0$, and a non-zero p is induced by the external field σ

$$\left.\begin{aligned} p_z &= \chi_\parallel \sigma_{xx}, \\ p_\alpha &= \chi_\perp \sigma_z^\alpha; \end{aligned}\right\} \tag{27}$$

$\chi_\parallel$, $\chi_\perp$ are the polarizabilities parallel and perpendicular respectively to the column axis. From equations (25) and (27) we obtain effective elastic constants

$$\left.\begin{aligned} B^{\mathrm{eff}} &= B/(1 + \chi_\parallel B), \\ C^{\mathrm{eff}} &= C/(1 + \chi_\parallel B), \\ K_3^{\mathrm{eff}}(\mathbf{q}) &= K_3/(1 + \chi_\perp k_3 q_z^2). \end{aligned}\right\} \tag{28}$$

In the dilute regime, it is clear that $B\chi_\parallel \propto \phi$ so that no spectacular effect is expected. The concentration regime (if attainable), and with $n(l)\,dl \propto a^{-2}\bar{l}^{-2}\exp(-l/\bar{l})\,dl$ (where $n(l)\,dl$ is the number of segments of length between l and $l + dl$ per unit volume) does not give much more spectacular results. For instance, if we consider, polymer-like segments, we can write the change in free energy of a segment [10] as

$$\Delta w = \tfrac{3}{2}kT\frac{z^2}{R^2} - \sigma_x^x a^2 z \tag{29}$$

in which R is the gyration radius: $R^2 = al$. Hence, minimizing with respect to z, we find

$$z(l) = \frac{a^3 l}{k_{\mathrm{B}}T}\sigma_x^x \tag{30}$$

and

$$p_z = \int_0^\infty z(l)a^2 n(l)\,dl = \frac{a^3}{k_{\mathrm{B}}T}\sigma_x^x, \tag{31}$$

which leads to $B\chi_\parallel \sim 1$.

If we consider the opposite limit in which the lines are essentially in the x, y plane, because of anisotropic line tension γ_{a}, we can write

$$\Delta w = \tfrac{1}{2}\gamma_{\mathrm{a}} l\alpha^2 - \sigma_x^x a^2 z, \tag{33}$$

where α is the tilt angle of the line with respect to the x, y plane. In this limit $\alpha = zl$, hence $z = la^2\sigma_x^x/\gamma_{\mathrm{a}}$ after minimization, this relation is similar to equation (30) provided we replace kT/a by γ_a. Thus $B\chi_\parallel \sim Ba^2/\gamma_a$ which may be larger than one if $(\gamma_a/a^2) \ll B$, but never very large, since for vanishing γ_a we would recover the polymer limit.

This shows that an important decrease of B and C can take place only in a regime in which the density of column extremities is very high. It is then likely that dislocations come in, which leads probably to a dislocation melting picture of the Nelson–Toner type [11]. We should not however discard the possibility of ionization of the column extremities via a discontinuous process.

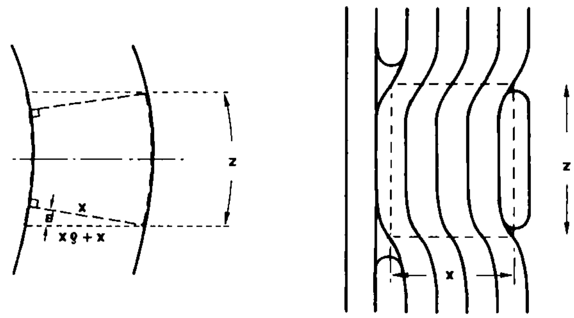

Figure 3. In the absence of permeation, the curvilinear length z can be considered as constant (i.e. an incompressible fluid). This necessitates an increase in the length of the lock-in fault segment: $\delta x = \frac{1}{2}\beta x^2 = \frac{1}{8}z^2 x[(\partial/\partial z)m_x^z]^2$.

The bending modulus behaviour is more interesting in the absence of permeation. Equalities (28) show that K_3 is not modified in the long wavelength limit. K_3 must then be calculated at fixed line configurations. Since these lines connect bunches of columns, we expect an increase in the bending modulus, compared to the nematic values. In the following we propose only very approximate arguments which have no pretence of being rigorous. We replace the complex ensemble of polydisperse segments by a monodisperse quadrilateral of width x and height z (z is the average size of a column). Bending such a system necessitates a tilt $\beta = (z\partial/2\partial z)m_x^z$ of the lines with respect to the columns normal and an increase (see figure 3)

$$\delta x = \tfrac{1}{8}z^2\left(\frac{\partial}{\partial z}m_x^z\right)^2 x. \tag{34}$$

Hence a free energy increase (in the limit of rigid lines) is given by

$$\delta W = \gamma_a x\beta^2 + 2\gamma\,\delta x, \tag{35}$$

$$\delta W = \left(\frac{\gamma_a + \gamma}{4}\right) xz^2\left(\frac{\partial}{\partial z}m_z^x\right)^2 \tag{36}$$

and an elastic constant

$$K_3^{\text{eff}} \simeq \left(\frac{\gamma_a + \gamma}{2}\right) xz^2 n \tag{37}$$

(where n is the number of quadrilaterals per unit volume). With $n \simeq \Phi/[2a^2(z + x)]$ in which Φ is the volume fraction of quadrilaterals we obtain

$$K_3^{\text{eff}} \simeq \frac{\gamma_a + \gamma}{4}\,\frac{rz^2}{(x + z)a^2}\,\Phi. \tag{38}$$

This estimate suggests a very large increase of the bend modulus. Taking $(\gamma_a + \gamma) \approx 10^{-5}$ dyn, $x \simeq z \simeq 10^{-5}$ cm, $a \simeq 3 \times 10^{-7}$ and $\Phi \approx 0{\cdot}1$ gives $K_3 \approx 10^{-2}$ dyn. This is an enormous value compared to that for nematic, but it is indeed compatible with the Orsay experiments [12].

5. Discussion

The lock-in fault lines are original, topologically stable defects, which can be described in terms of dislocation dipoles just like dislocations may be thought of as disclination dipoles; they can end on point defects. This situation is analogous to that corresponding to the Dirac monopoles. The most interesting consequence, in the absence of permeation, an anomalous increase of the bend modulus of several orders of magnitude as compared to the nematic value. This is a plausible explanation of the enormous K_3 values found at Orsay [12].

The estimate we propose here is very approximate: we should obviously take account of the distribution of lines, and also of dislocations, but we believe that it keeps the essential physics. It would be interesting to try to provide experimental evidence for the column extremities and the lock-in fault lines. This could be achieved by direct observation with electron microscopy and by looking for their signature in X-ray diffraction patterns. Vortex states in type two superconductors have the same columnar structure. Topological defects are very similar, but because of the absence of magnetic dipoles, there are neither vortex extremities nor edge dislocations. Screw dislocations and lock-in fault lines are allowed.

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