

A feature of two-dimensional first-order phase transitions in planar defects in crystals

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Two-dimensional first order phase transitions can occur either in thin liquid (crystal) films or in planar defects within crystals, such as grain boundaries, twinning boundaries, or stacking faults. At the surfaces of liquids and crystals these transitions are not possible because of electrocapillary¹ and striction² effects, respectively. In films the interface between the different states that coexist at the transition point has a finite energy (per unit length); this corresponds to a classical first-order phase transition. An essentially different picture should be seen in a planar defect in the volume of a crystal.

Let us consider, e.g., a phase transition in a planar stacking fault. In each of the states coexisting at the transition point the stacking fault must have a different thickness b_1 and b_2 (see Fig. 1). Therefore, in the volume of the crystal, around the boundary line between the phases there will be a strain field characteristic of an edge dislocation. In this case the difference $b_1 - b_2$ plays the role of the Burgers vector. As is known (see, e.g., Ref. 3) the energy of the dislocation has a logarithmic divergence and in a cylindrical region of radius R around the dislocation in an isotropic crystal it is equal to

$$\frac{E(b_1 - b_2)^2}{8\pi(1 - \sigma^2)} \ln \frac{R}{a} \quad (1)$$

per unit length. Here a is a quantity by the order of an atomic spacing, E is Young's modulus, and σ is the Poisson ratio.

In addition to the positive energy (1) there is a negative contribution² resulting from the surface tension:

$$- \frac{(\beta_1 - \beta_2)^2 (1 - \sigma^2)}{2\pi E} \ln \frac{R}{a}; \quad (2)$$

where β_1 and β_2 are the surface-tension coefficients in phases 1 and 2. A first-order phase transition, clearly, is possible only if the sum of the contributions (1) and (2) is positive.

Let us assume that the first phase is in a metastable state near the transition point. The energy α_1 per unit

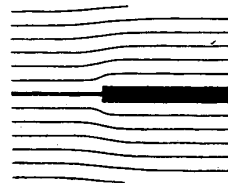


FIG. 1

area of a planar stacking fault in this state is somewhat greater than its energy α_2 in the second state. The energy of formation of a nucleation center of phase 2 is then

$$(\alpha_2 - \alpha_1) \pi R^2 + A \cdot 2\pi R \ln \frac{R}{a} \quad (3)$$

where R is the radius of the nucleation center and A is the sum of the coefficients multiplying the logarithms in (1) and (2). Let us write down the results obtained from (3) for the size of a critical nucleus

$$R_c = \frac{A}{\alpha_1 - \alpha_2} \ln \frac{A}{a(\alpha_1 - \alpha_2)} \quad (4)$$

and its energy

$$E_c = \frac{\pi A^2}{\alpha_1 - \alpha_2} \ln \left[\frac{A}{a(\alpha_1 - \alpha_2)} \right]^2 \quad (5)$$

If the value of A is small in comparison with the intrinsic energy γ per unit length of the phase-boundary line [when the usual term $2\pi R\gamma$ should be added to (3)], then the anomalous expressions (4) and (5) will apply only in the immediate vicinity of the transition point as long as

$$\alpha_1 - \alpha_2 \ll \frac{A}{a} \exp \left(- \frac{\gamma}{A} \right)$$

It is clear that the dislocation effect being considered occurs in any plane defect in the volume of the crystal. We also note that the limitations² on the symmetry of plane defects and the conclusion of Ref. 2 that parquet-type structures can exist are still valid, since the equiv-

alent states considered in that paper clearly have the same thickness.

¹V. I. Marchenko, *Zh. Eksp. Teor. Fiz.* **81**, 1141 (1981) [*Sov. Phys. JETP* **54**, 605 (1981)].

²V. I. Marchenko, *Pis'ma Zh. Eksp. Teor. Fiz.* **33**, 397 (1981) [*JETP Lett.* **33**, 381 (1981)].

³L. D. Landau and E. M. Lifshitz, *Theory of Elasticity*, 2nd Ed., Pergamon Press, Oxford (1970).