Topological order of the structure of atomically rough crystal boundaries

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There are three types of atomically rough states of crystal surfaces. Two of them are characterized by topological order. Unique phase transitions should occur between these states.

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At zero temperatures, thermal equilibrium corresponds to strict ordering of the positions of atoms on each face of a classical crystal. The orientation of all faces is determined

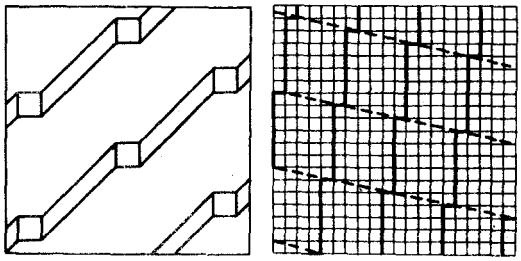

FIG. 1. a) Face close to the (1*N*0) face; b) its projection on the (010) plane.

by the Miller indices, and thus the surface energy is a function that is defined at rational points. As shown by Landau,[1] this circumstance, as well as the fact that on such surfaces there exist special topological defects, namely, steps, is related to the unique nonanalytic dependence of the surface energy on the orientation of a face. The situation qualitatively changes at finite temperatures in connection with the appearance of atomically rough surfaces.

We shall examine faces close to the direction (1*N*0) of a simple cubic lattice (Fig. 1). Such faces have only translational symmetry. For simplicity, we shall discuss the faces on which the distance between the breaks at the steps are identical and equal to K lattice constants. The surface defect, which has a minimum energy, is the displacement of a single break by one atomic distance (i.e., the removal or addition of one atom). If K, $N \gg 1$, then this energy is small, since it is due to the elastic interaction of steps, decreasing rapidly with distance, ($\propto R^{-2}$) and breaks ($\propto R^{-3}$).[2] Clearly, if the temperature is greater than this energy, then the translational order in the lattice consisting of breaks cannot be maintained. It is evident, however, that topological order, which is characteristic for the usual two-dimensional crystals (Fig. 2a), remains. In this case, the square of the displacement of each break diverges logarithmically with the dimension of the face, but the relative distances between neighbors fluctuate little, so long as the temperature is small compared to their interaction energy. Here, only a single component of the displacement vector v (along the steps) is meaningful, so that the stress energy density reduces to the expression

$$\lambda_1\left(\frac{\partial v}{\partial x}\right)^2 + \lambda_2\left(\frac{\partial v}{\partial y}\right)^2 + \lambda_3\frac{\partial v}{\partial x}\frac{\partial v}{\partial y}, \tag{1}$$

from which it is clear that the correlation function has a form characteristic for the usual two-dimensional crystals.[3]

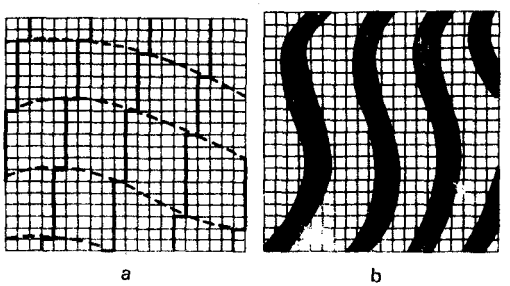

Fig. 2. a) Atomically rough surface of type I; b) atomically rough surface of type II.

Because of the developed fluctuations, all characteristics along separate regions, which are faces with different definite Miller indices, are statistically averaged for the orientation of the surface examined. It is clear that after such averaging all orientations of the surface (rather than only those related to rational numbers) are important and the surface energy becomes an analytic function of the angle. This is the basic property of an atomically rough surface.

We note that a phase transition from an atomically smooth to an atomically rough state, for the example examined, turns out to be essentially the same phenomenon as a transition from a commensurate to an incommensurate state, where a continuous degree of freedom also appears.

As the temperature is increased, as in the usual two-dimensional crystal, a phase transition destroying the topological order must occur. However, it is not related to the Kosterlitz-Thouless instability,[4] since a crystal consisting of breaks has no dislocations. Indeed, each dashed line, drawn through the breaks in Fig. 2a, is nothing more than a step on the (1N0) face. On the other hand, the step cannot have an end, which is necessary for creating dislocations. We can say that the transition occurs when these steps "swell" due to thermal fluctuations, and their width becomes equal to the distance between them, i.e., the steps lose their individuality. The transition is necessarily a second-order transition, since first-order transitions on crystal surfaces are generally impossible due to striction effects.[5]

After the phase transition, the breaks on different steps are not correlated with each other. Each step transforms into a one-dimensional system, which can be described by averaged, with respect to fluctuations in the positions of the breaks on it, characteristics. The steps cannot come close to each other due to elastic repulsion. Thus, there arises a new II atomically rough state (Fig. 2b) with the topology of a two-dimensional smectic liquid crystal. If the question in phase I is one of fluctuations in a series of steps on the (1N0) face, then the question in phase II is one of fluctuations in a series of steps on the (010) face. The deformation energy of phase II for this reason, in contrast to the usual smectic, is again determined by expression (1); the elastic constants, however, are much greater [if we assume that $N \sim K$, then they are greater roughly speaking by a factor of N, which is clear, if we compare the change in the surface energy accompanying a change in the distance between the steps (N) by a factor of 2 and with the same change in distance between breaks (K)].

With a further increase in temperature, there must occur a phase transition, which is of the same nature as the transition I $\rightarrow$ II and there arises an atomically rough state III of a type without topological order. It is clear that this transition accompanies the transition of the atomically smooth-atomically rough state on the (010) face because for large N the steps on the (010) face lose their individuality on the (1N0) face almost at the same time as the step on the (010) face breaks down.

The states I and II do not form on all faces. Thus, on the (010) face, there is a transition from an atomically smooth to a rough state of type III. On the (1N0) faces there is no I phase; the transition occurs immediately to phase II due to the appearance of a certain number of thermally active pairs of breaks on the steps: The situation here is completely analogous to a system of chains consisting of adsorbed atoms.[6] If a pair of breaks with opposite sign is formed on one of the steps and they are separated by a distance n

$\gg N$, then an attraction appears between breaks $\sim nT_0/N^3$ due to repulsion of steps $\sim T_0/N^2$ [T_0 is of the order of the temperature of the transition to the rough state of the (010) face], ("quarks do not escape"). Equating the average value $\langle n\rangle \sim TN^3/T_0$ to the average distance between the pairs of breaks $\sim \exp(T_0/T)$, we obtain an estimate of the temperature at which the ($1N0$) face undergoes a transition to the rough state $\sim T_0/\ln N$ (compare Ref. 6). The transition to phase I is estimated analogously.

The reasoning above is applicable near any atomically smooth face, since the concepts of step and break are defined on each such face. For example, a step on a ($1N0$) face is a break in the distance between steps on the (010) face: $\ldots, N, N, N \pm 1, N, N, \ldots$. If we now examine a face close to ($1N0$), consisting of these steps, and in addition the distance between them is equal to LN, then the temperature of the transition to the rough state is of the order of $T_0/\ln(LN)$. A smectic with period LN is obtained and, further, for temperatures close to $T_0/\ln N$, a phase transition occurs to the smectic with a period close to N.

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