Steps on the surfaces of quasicrystals

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It is shown that the surfaces of quasicrystals can exist in an atomically smooth state. The energy of the elementary steps on such a surface has a logarithmic divergence.

The possibility of a face of an ordinary crystal existing in an atomically smooth state is due to the periodicity of the crystal in the direction perpendicular to the boundary. The same is true, as will be shown in the present note, for a quasicrystal. Since the symmetry of the quasicrystals is higher than that of crystals, the atomically smooth state in quasicrystals has a number of interesting features. The height of the steps can assume any one of a discrete, infinite set of incommensurate values, and their energy has a logarithmic divergence (this is characteristic of dislocations).

Let us consider the simplest possible quasicrystalline structure—a two-dimensional quasicrystal with an eight-order axis. The symmetry of the structure is determined by the Fourier components of the spatial modulation of the density function $\rho(\mathbf{r})$:

$$\rho(\mathbf{r}) = \rho_0 + \sum |\rho_{\mathbf{k}}| e^{i(\mathbf{kr} - \varphi_{\mathbf{k}})} . \tag{1}$$

The deformations of the quasicrystal are described by four phase fields φ_1, φ_2, φ_3, φ_4, corresponding to the principal harmonics with minimal wave vectors in absolute value oriented at angles of $\pi/2$ and $\pi/4$ with respect to each other (see Fig. 1). By virtue of the fact that the density is real-valued, $\varphi_{\mathbf{k}} = -\varphi_{-\mathbf{k}}$.
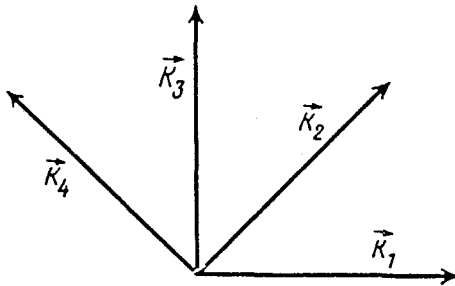
We introduce the complex fields

$$u_x + i u_y = \frac{a}{2\pi}(\varphi_1 + e^{i\pi/4}\varphi_2 + e^{i2\pi/4}\varphi_3 + e^{i3\pi/4}\varphi_4)$$

$$\xi + i\chi = \frac{a}{2\pi}(\varphi_1 + e^{i3\pi/4}\varphi_2 + e^{i6\pi/4}\varphi_3 + e^{i9\pi/4}\varphi_4) . \tag{2}$$

The components u_x and u_y form the displacement vector of the quasicrystal as a whole, and the quantities ξ and χ correspond to the so-called internal phase motion; the x axis is directed along the vector $\mathbf{k}$, and the y axis, along the vector $\mathbf{k}_3$. Note that the quantities ξ and χ can be considered as the countermotion field of two lattices, one of which is constructed from the vector pair $\mathbf{k}_1$, $\mathbf{k}_2$, and the other, from the pair $\mathbf{k}_3$, $\mathbf{k}_4$. Here ξ corresponds to such a motion along the x axis, and χ corresponds to the motion along the y axis.

Let the surface of the quasicrystal be oriented along the vector $\mathbf{k}_1$. Extension of the results obtained below to other possible orientations does not cause any fundamental difficulties, but for the sake of an example this is the simplest case. The state of the quasicrystal changes, but its bulk energy remains the same upon the addition to each of its phases of the constant increments $\delta\varphi_i$. There is no basis, however, for assuming that its surface energy does not change during such a transformation. Indeed, if we vary the quantity χ, corresponding to the countermotion of the two above-indicated lattices along the surface normal, then the surface energy should vary. It is clear that the structure of the boundary and, in particular, its effective thickness, cannot remain constant during such motion. The minimum of the surface energy corresponds to some completely determined value of χ, and nothing prevents us from assuming that this value of χ is zero. For the quantity ξ and the displacement vector $\mathbf{u}$ there is no such condition fixing their values. Thus, for the equations of equilibrium, which describes some deformed state of the quasicrystal, we have natural boundary conditions in $\mathbf{u}$ and ξ—the absence of the corresponding stresses, and the variable χ should be equal to zero.

In ordinary crystals the set of energy-equivalent states of the boundary is obtained by incrementing the integral number of atomic planes. In quasicrystals the corresponding set for the boundary under consideration is formed by increasing the height of the quasicrystal

$$h = a(N + \sqrt{2}M) \tag{3}$$

with a simultaneous phase shift

$$\chi = a(N - \sqrt{2}M); \quad \xi = u_x = u_y = 0 \ , \tag{4}$$

where N and M are integers. The density function (1) in coordinates reckoned from the position of each of these boundaries will be the same for each of them. It is just this property that is necessary to ensure the possibility for the existence of an atomically smooth state. Since in the transition from one possible state to another it is necessary to perform the phase transformation (4), deformations should appear near a step in the bulk of the quasicrystal which are characteristic of dislocations.

The phase deformation energy of the quasicrystals[1] of the given symmetry reduces to the following expression [see Eq. (6) in Ref. 2]:

$$\lambda_1(\partial_x + i\partial_y)(\xi + -i\chi)(\partial_x - i\partial_y)(\xi - i\chi) + \lambda_2(\partial_x + i\partial_y)(\xi - i\chi)(\partial_x - i\partial_y)(\xi + i\chi)$$

$$+ \lambda_3\{(\partial_x + i\partial_y)(\xi + i\chi)(\partial_x + i\partial_y)(\xi + i\chi) + \text{c.c.}\} \ . \tag{5}$$

Limiting the discussion to the demonstration of the dislocation effect, we will disregard the cross terms and the ordinary elastic degrees of freedom. Only phase deformations will then appear near a step. These phase deformations are described by the equation

$$a\Delta\xi + (\partial_x^2 - \partial_y^3)\xi - 2\partial_x\partial_y\chi = 0 \; ; \quad a\Delta\chi - (\partial_x^2 - \partial_y^2)\chi - 2\partial_x\partial_y\xi = 0 \; , \tag{6}$$

where $a = (\lambda_1 + \lambda_2)/2\lambda_3$, and by the boundary conditions on the surface $y = 0$: the condition of the absence of tangential phase ξ-stresses

$$(\alpha - 1)\partial_y\xi + (\beta - 1)\partial_x\chi = 0 \; , \tag{7}$$

where $\beta = (\lambda_1 - \lambda_2)/2\lambda_3$, and the conditions fixing the phase shift χ during the transition from one side of the step $x < 0$ to the other $x > 0$:

$$x < 0 : \quad \chi = 0; \; x > 0 : \quad \chi = b = a(N - \sqrt{2}M) \; . \tag{8}$$

The solution of problem (6)–(8) can be easily found by making use of the obvious analogy with an edge dislocation (see Ref. 3, Problem 4 in §27):

$$\xi = -\frac{b}{\pi}\ln\sqrt{x^2 + y^2}; \quad \chi = \frac{b}{2} + \frac{b}{\pi}\arctan\frac{x}{y} \; . \tag{9}$$

The step energy is

$$\frac{4}{\pi}\lambda_2 b^2 \ln\frac{L}{a} \; , \tag{10}$$

where the length L is of the order of the dimension of the sample; if it is a step with opposite sign, then it is of the order of the distance between the steps.

This result leads to a number of obvious consequences for the properties of quasicrystals.

First, at low enough temperatures, in their equilibrium shape the quasicrystals should present only a few faces. It is not possible, all the same, to exclude a striction instability of the edges,[4] upon which the faces will join with rounded sections.

Second, the growth of the atomically smooth face should take place by means of the generation and growth of new layers—completely similar to the layer-by-layer mechanisms of growth of atomically smooth faces of crystals. Here, however, the problem is substantially complicated by the appearance of steps of different height and by the character of the step energy. Here the main difficulty is not with the logarithm, but with the dependence of the quantity b on the numbers M and N, which define the step parameters.

Third, the phase transition to an atomically rough state should differ substantially from such a transition on the surface of a crystal.

Fourth, on the surfaces of quasicrystals two-dimensional first-order phase transitions are not forbidden, as is the case with crystals and liquids, since the discovered "phase logarithm" arises at the boundary of two-dimensional surface phases and competes with the instabilities indicated in Refs. 4 and 5. However, the kinetics of such a transition has its own peculiarities.[6]

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