Ground state of a d-dimensional elastic crystal in an incommensurate d-dimensional periodic potential

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The ground state of a d-dimensional elastic crystal, which has a cubic symmetry and which is in a d-dimensional periodic square potential having the same symmetry but incommensurate lattice constants and potentials, has been determined. For the case $d \geqslant 2$ an abrupt transition in the incommensurateness parameter from the commensurate phase to the modulated phase has been found.

The description of structures which are produced as a result of competition between two or more dimensions for different dimensionalities (epitaxial films on single-crystal substrates, $d=2$; formation and growth of nucleation centers in phase transitions, $d=3$; and others) remains an important problem in solid-state physics. In the case of epitaxy of crystalline films on incommensurate single-crystal substrates or in the case of equilibrium growth of crystals on single crystals, the following growth picture is observed: A heteromorphic phase, in which the structure of the grown crystal adjusts completely to the structure of the substrate, forms initially. Then, on the basis of the crystal and substrate, a weakly deformed crystal, having the initial characteristic dimensions of the crystal lattice and symmetry, forms abruptly. This process, well known to experimentalists, has not yet been given a sufficiently simple theoretical explanation, probably because the theoretical descriptions of such structures have usually been based on one-dimensional models.[1,2] Furthermore, the mathematical apparatus used for describing modulated structures with a potential of arbitrary form is complicated, even in the one-dimensional case. It would therefore be worthwhile to consider a multidimensional model, after simplifying it as much as possible, in particular, after retaining only one incommensurateness parameter and choosing the simplest potential.

The one-dimensional system ($d=1$) consisting of an elastic chain of atoms in a periodic potential, whose period is incommensurate with the period of the chain, has been studied extensively and the ground state of such a system is well known.[1,2] The ground state is especially simple for a square potential (Fig. 1), in which chain atoms can be pinned only at the walls of the potential. In this case the solution modulated with a period $1/\rho$ has only two independent parameters—the number $N\rho L$ of atoms in the region of the potential wells and the number $M\rho L$ of atoms in the region of the potential barriers, where L is the total number of atoms in the chain and $\rho=1/(N+M)$. The ground state is found by varying the potential energy of the system with respect to these parameters. Let the size of the potential well be equal to the size of the barriers, assumed to be unity, and let the period of the chain be equal to $2+\delta$, where $\delta \ll 1$. If the potential $V(r)$ is given by the function

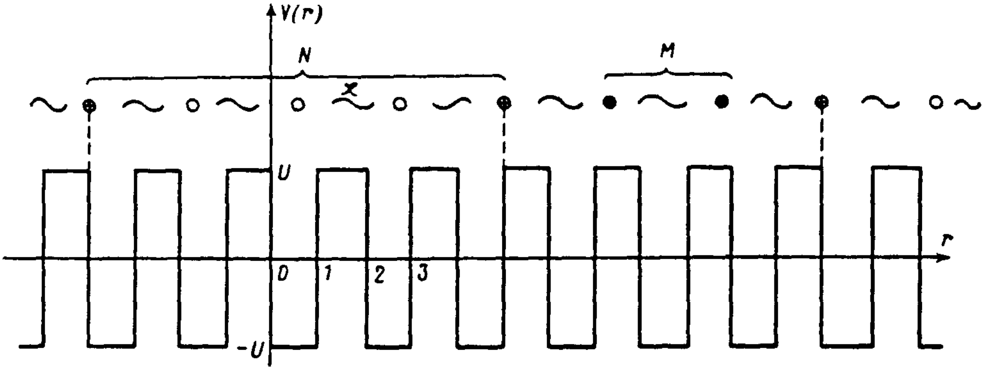

FIG. 1.

$$V(r)=\begin{cases} -U & \text{—inside the potential wells} \\ 0 & \text{—at the well-barrier boundaries}, \\ U & \text{—near the potential barrier} \end{cases} \tag{1}$$

then the total energy E of the one-dimensional system can be written, as one can see from Fig. 1, in the form

$$E=-U\frac{(N-M-2)}{N+M}L+\frac{\kappa}{2}[(N-1)(\delta-\delta_1)^2(M+1)(\delta-\delta_2)^2]\frac{L}{N+M}, \tag{2}$$

where κ is the elastic constant of the chain, $\delta_1=1/(N-1)$, and $\delta_2=1/(M+1)$. Making the substitutions $x=N-1$, $y=M+1$, and $U/\kappa=\delta_c^2$, we rewrite Eq. (2) in the form

$$\epsilon=\frac{2E}{\kappa L^d}=\delta^2-2\delta_c^2\frac{(x-y)}{x+y}-\frac{4\delta}{x+y}+\frac{1}{xy}, \quad x>0, \quad y>0. \tag{3}$$

Expression (3) for the energy density ϵ can be extended to the d-dimensional case as follows:

$$\epsilon=\frac{2E}{\kappa L^d}=d\delta^2-2\delta_c^2\frac{(x-y)^d}{(x+y)^d}-d\frac{4\delta}{x+y}+d\frac{1}{xy}, \quad x>0, \quad y>0, \tag{4}$$

which can be easily verified independently for the example $d=2$ (Fig. 2). Analyzing ϵ in Eq. (4) for local minima as functions of the two variables x and y, we obtain two solutions. The first solution has the form

$$x=\xi/\delta(\xi-1), \quad \xi=(\delta_c/\delta)^{2/(d-2)}$$

$$y=\xi/\delta(\xi+1), \quad x>0, \quad y>0; \tag{5}$$

$$\epsilon=(d-2)\delta^2/\xi^2;$$

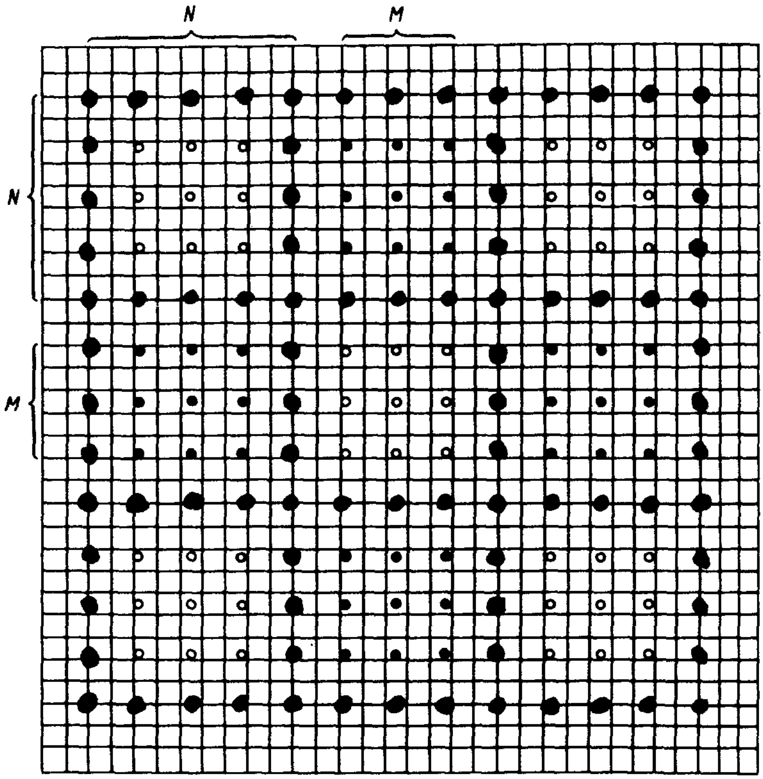

FIG. 2. Qualitative illustration of the ground state of the crystal ($d=2$, $\delta=1/4\geqslant\tilde{\delta}_c$), where ○ is a crystal atom inside a potential well, • is a crystal atom inside a potential barrier, and ● is a crystal atom on the well-barrier boundary.

and the second solution has the form

$$x=y=1/\delta,$$
$$\epsilon=0. \tag{6}$$

In addition, there exists the limiting solution $x=L\to\infty$, which describes the commensurate phase (uniformly compressed crystal) with the energy

$$\epsilon_0=d\delta^2-2\delta_c^2. \tag{7}$$

Comparing ϵ in Eq. (5) with ϵ_0, we conclude that solution (5) is realized only for $d=1$ and $\delta\geqslant\delta_c$. In this case the transition in the incommensurateness parameter δ from the commensurate state with $\rho=0$ to the modulated state is discontinuous at the point $\delta=\delta_c$. Comparing ϵ in Eq. (6) to ϵ_0, we conclude that for $d\geqslant2$ a first-order phase transition in the parameter δ occurs at the point $\delta=\tilde{\delta}_c=(2/d)^{1/2}\delta_c$ and ρ changes abruptly from $\rho=0$ to $\rho=\tilde{\delta}_c/2$. The energy was minimized in the class of simple modulated solutions and under the assumption that the elastic bonds of the atoms of the crystal are orthogonal. Consideration of other solutions, in particular, solutions modulated only in a single direction, does not lead to new results. Since the potential $V(r)$ in Eq. (1) is nonanalytic and degenerate, the solution for the ground state with $\delta \geqslant \widetilde{\delta}_c$ is identical to the solution for the underformed crystal (Fig. 2). In general, the crystal with $\delta \geqslant \delta_c$ is deformed and modulated with a period $2/\delta$ with an insignificant change in its linear dimensions. The commensurate (heteromorphic) phase of a uniformly compressed crystal is realized if $\delta < \widetilde{\delta}_c$, with

$$\epsilon_0 = d\delta^2 - \frac{2}{\kappa} V_{\min}(r), \tag{8}$$

where $V(r)$ is a generalization of the potential (1). Let us examine the first term in Eq. (8), which is proportional to d. For an analytic periodic potential $V(r)$ the threshold value of the parameter $\delta = \widetilde{\delta}_c$ should decrease, since in this case there is an additional possibility for the crystal atoms to adjust themselves to the potential. The extension of the model to an arbitrary case apparently will not change fundamentally the overall picture of the solution obtained, except for $d = 1$, where taking into account the analyticity and the finite elasticity of the potential leads to an asymmetric (with respect to the sign of δ) phase transition.[3] Furthermore, a point of interest here is also the fact [Eq. (8)] that in the limit $d \to \infty$ the region corresponding to a commensurate phase is virtually nonexistent with respect to the parameter δ. Returning to experiment, we note that an increase in the layers of the crystal grown corresponds to an increase in κ in our model and therefore a decrease of $\widetilde{\delta}_c$. For a definite thickness of the film, δ becomes greater than $\widetilde{\delta}_c$, and the crystal should transform abruptly into a weakly deformed state, as does actually happen in practice.

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[1] F. C. Frank and I. H. van der Merwe, Proc. Roy. Soc. **198**, 205 (1949).
[2] V. L. Pokrovskii and A. L. Talapov, Zh. Eksp. Teor. Fiz. **75**, 1151 (1978) [Sov. Phys. JETP **48**, 579 (1978)].
[3] A. N. Filonov, Fiz. Tverd. Tela **30**, 28 (1988) [Sov. Phys. Solid State **30**, 15 (1988)].

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