Incommensurate system on a deformable substrate

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An exact solution describing a system of adsorbed atoms on a deformable crystalline substrate is found. It is shown that the deformation of the substrate gives rise to a correction to the repulsion energy of the solitons that arise in the incommensurate phase. This correction, which does not depend on the form of the atom-substrate interaction potential, is always positive, and, as a result, the transition into the incommensurate phase is of second order.

Recently there has been an upsurge in interest in the study of monatomic films of different materials adsorbed on crystalline substrates. Transitions from the commensurate into the incommensurate state have been experimentally observed in such films.[1-4] A number of theoretical papers[5-7] have been devoted to the transition into the incommensurate phase. In these papers it is assumed that the crystalline substrate is so rigid that it is not deformed by the forces exerted on it by the adsorbed atoms. It is shown that, in the incommensurate phase and near the transition point, almost all the atoms are located very close to the minima of the substrate potential. But there are regions, called soliton lines, where the atoms are appreciably displaced from these minima. If the energy characterizing the interaction between the atoms and the substrate is much smaller than the characteristic energy of the elastic interaction between the atoms, the width of the soliton lines is many times greater than the lattice constant. Therefore, elasticity theory can be used to describe the distortions of the adsorbed-atom lattice.

Various relative dispositions of the soliton lines are possible. In particular, a structure consisting of parallel soliton lines spaced L apart is possible. The energy per unit area of such a structure is equal to

$$E = [-A(\delta-\delta_c) + B \exp(-L/l_s)]/L, \qquad (1)$$

where $A, B > 0$ are some constants, l_s is the soliton-line width, and δ is a linear function of the chemical potential of the atoms. The quantity $A(\delta_c - \delta)$ is the self-energy per unit length of a soliton line. It vanishes at the commensurate–incommensurate (C–I) transition point, where $\delta = \delta_c$. The second term in (1), i.e., the term containing $\exp(-L/l_s)$, describes the repulsion of the solitons that arise in the region $\delta > \delta_c$.

Minimization of (1) with respect to L leads to the following dependence of the soliton spacing on δ:

$$L \sim l_s \ln [\delta_c/(\delta-\delta_c)]. \qquad (2)$$

Gordon and Villain[8] have noted that allowance for the deformability of the substrate leads to the appearance of an additional contribution, equal to C/L^3 (where C is some constant), to the energy E of the soliton lattice. If $C < 0$, then the C–I phase transition should be of first order. If, on the other hand, $C > 0$, then $L \sim (\delta - \delta_c)^{-1/2}$ in the vicinity of the C–I phase transition point.

The experimental observation of the structure consisting of parallel soliton lines has been reported by Jaubert *et al.*,[4] who studied the behavior of Xe adsorbed on the (110) face of copper. This face is prepared as follows. It has troughs in the x-axis direction. The Xe atoms are located in these troughs. The distance between the atoms in the x direction changes during the transition into the incommensurate phase, while the spacing in the perpendicular (y) direction remains unchanged with high degree of accuracy. Therefore, the structure of the incommensurate phase can be characterized by the displacement $\varphi(x)$ of the Xe atoms along the x axis from those positions which they occupied in the commensurate phase. For the systems in which the atoms in the incommensurate phase are displaced only in one direction, we shall compute exactly the contribution to the energy E, due to the deformation of the substrate.

At zero temperature, the total energy of the deformable substrate and of the system of adsorbed atoms interacting with it can be written in the form

$$H = \int \left[\frac{K}{2}\left(\frac{\partial\varphi}{\partial x}\right)^2 - K\delta\frac{\partial\varphi}{\partial x} + V(\varphi - u_x(z=0)) \right] dx\, dy + \int \left[\frac{\lambda_x}{2}\left(\frac{\partial u_x}{\partial x}\right)^2 \right.$$
$$\left. + \frac{\lambda_z}{2}\left(\frac{\partial u_z}{\partial z}\right)^2 + \lambda_{xz}\frac{\partial u_x}{\partial x}\frac{\partial u_z}{\partial z} + \frac{\mu}{2}\left(\frac{\partial u_z}{\partial z} + \frac{\partial u_z}{\partial x}\right)^2 \right] dx\, dy\, dz, \qquad (3)$$

where the first integral is over the surface and the second is over the volume of the substrate. In the formula (3) K is the elastic constant of the adsorbed-atom lattice; δ is a linear function of the chemical potential of the atoms; λ_x, λ_z, λ_{xz}, and μ are the elastic constants of the substrate; and u_x and u_z are the components of the displacement of the substrate atoms. The use of elasticity theory is legitimate when the atom-substrate interaction potential V is small compared to the characteristic elastic energies, i.e., if

$$|V| \ll K, \quad K \lesssim \lambda b, \mu b, \qquad (4)$$

where b is the lattice constant of the substrate. Under the conditions (4), we can write V in the form of a periodic function of the argument $[\varphi - u_x(z=0)]$.

Let us first consider the particular case in which the energy (3) can be computed exactly. Let V, as a periodic function of its argument α, have the form shown in Fig. 1, i.e., let

$$V(\alpha) = \varkappa\alpha^2/2 \text{ for } |\alpha| \leq b/2, \qquad (5)$$

and let the function $V(\alpha)$ for the remaining values of α be obtainable by periodic continuation with period b. A potential of this form is used in Ref. 5.
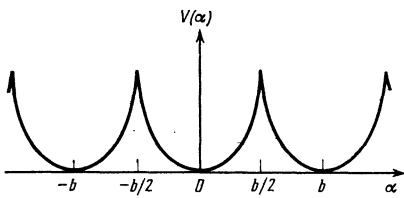
FIG. 1.

We shall seek the solution to the equilibrium equations, in which $\partial\varphi/\partial x$ and u_x, u_z are periodic functions of the coordinate x with period L. The equilibrium equations are solved with the aid of the Fourier transformation procedure. The energy per unit length of a soliton line turns out to be

$$E_s = \frac{Kb^2}{2L} \sum_{n=-\infty}^{+\infty} \left(1 + \frac{K}{\varkappa}k_n^2 + \frac{K}{\lambda}|k_n|\right)^{-1} - K\delta b, \qquad (6)$$

where $k_n = 2\pi n/L$ and

$$\frac{1}{\lambda} = \left(\frac{\lambda_z}{\mu}\right)^{1/2} \left[\frac{(\lambda_x\lambda_z)^{1/2}+\lambda_{xz}+2\mu}{(\lambda_x\lambda_z)^{1/2}-\lambda_{xz}}\right]^{1/2} \frac{1}{(\lambda_x\lambda_z)^{1/2}+\lambda_{xz}}. \qquad (7)$$

The sum in (6) can easily be computed for the region near the C–I phase transition point, where $L \to \infty$:

$$E_s = \frac{(\varkappa K)^{1/2}b^2}{4}\left[1 - \frac{(\varkappa K)^{1/2}}{\pi\lambda} + 2\exp\left(-\left(\frac{\varkappa}{K}\right)^{1/2}L\right)\right] - b\delta K + \frac{\pi}{6}\frac{(Kb)^2}{\lambda L^2}. \qquad (8)$$

This formula agrees with (1) if

$$\delta_c = \frac{b}{4}\left(\frac{\varkappa}{K}\right)^{1/2}\left(1 - \frac{(\varkappa K)^{1/2}}{\pi\lambda}\right), \quad l_s = \left(\frac{K}{\varkappa}\right)^{1/2}.$$

The last term in (8) gives the soliton-repulsion energy that arises as a result of the deformation of the substrate. This energy is always positive. Therefore, the C–I phase transition is of second order.

It follows from (8) that, for a given soliton-line spacing L, the contribution to the energy from the deformation of the substrate does not depend on the magnitude $\varkappa$ of the adsorbed atom–substrate interaction potential. This suggests that the soliton-repulsion energy E_d that arises as a result of the deformation of the substrate does not depend on the form of the adsorbed atom–substrate interaction potential V, and is equal to

$$E_d = \frac{\pi}{6}\frac{(Kb)^2}{\lambda L^2}. \qquad (9)$$

And, indeed, a computation of the energy per unit length of a soliton line by perturbation theory in $1/\lambda$ yields the energy (9) for a periodic potential $V(\alpha)$ of any form. But the dimensionless parameter of the perturbation theory in $1/\lambda$ is unknown. On the face of it, we could show that this parameter is equal to $K/\lambda b$. But we can, by expanding the sum over n in (6) in powers of $1/\lambda$, easily verify that the expansion proceeds in powers of the small parameter

$$\varepsilon = (K\varkappa)^{1/2}/\lambda \equiv K/\lambda l_s.$$

On account of the conditions (4), the soliton width l_s is much greater than the lattice constant b. Therefore,

$\varepsilon \ll 1$ even when $K \sim \lambda b$. It is natural for $\varepsilon = K/\lambda l_s$ to be precisely the expansion parameter, since the smaller the adsorbed atom–substrate interaction energy is, the smaller should be the corrections to the energy that arise as a result of the deformability of the substrate.

In spite of the fact that the corrections to the sum in (6) are always small, they give rise to an important qualitative effect. The reason is that the dominant, L-independent part of the sum in (6) is conceled out at the C–I phase transition point by the term containing δ.

For a periodic potential V of arbitrary form, the energy per unit area is equal to

$$E = [-A(\delta-\delta_c) + B\exp(-L/l_s)]/L + \pi(Kb)^2/6\lambda L^3, \qquad (10)$$

where A, B, δ_c, and l_s can be obtained from the formulas given in Ref. 7. The term in (10) exponentially small in L can be neglected in the region sufficiently close to the C–I phase transition point, and minimization of (10) with respect to L yields the estimate

$$L \sim (\delta-\delta_c)^{-1/2} \qquad (11)$$

instead of (2). Such a dependence of the mean distance between the solitons on $\delta - \delta_c$ is obtained when allowance is made for the thermal fluctuations on the undeformable substrate. The relation (11) was experimentally discovered by Jaubert et al.[4] Because of the fact that the Xe–Xe and Xe–substrate interaction potentials are not sufficiently well known, we cannot at present identify with certainty the cause of the relation (11) found by Jaubert et al.,[4] i.e., whether it is the thermal fluctuations or the substrate distortion.

In the case of a substrate that can be described by the isotropic elasticity theory, Lyuksyutov[9] has obtained by perturbation theory an energy of the form (9) in which λ is expressed in terms of the bulk modulus and Poisson's ratio.

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