Two-dimensional anisotropic crystals

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A model of two-dimensional incommensurate crystals that describes the incommensurate structures formed in submonolayer films through compression of the commensurate structures along one of the substrate's crystallographic directions is considered. A self-consistent solution to the problem of the incommensurate crystal on an elastic substrate is obtained. It is shown that the interaction between the solitons via the elastic deformations of the substrate is determined not by the amplitude of the potential relief, but by the ratio of the elastic constants of the film and the substrate. The mechanism underlying the melting of the soliton lattice is investigated, and it is shown that the substrate-mediated elastic interaction alters the phase diagram. The dependence of the melting point and the Debye-Waller factor of the soliton lattice on the coverage is found.

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1. INTRODUCTION

Two-dimensional incommensurate crystals are the subject of intensive experimental and theoretical investigations (see Ref. 1 and the references therein). Theory predicts the presence of an acoustic mode in the vibrational spectrum of such a crystal despite the presence of the potential relief of the substrate. The experimental investigations of submonolayer films on metallic substrates have shown that the excitation spectrum of incommensurate structures indeed contains a gapless branch.[2] The number of different adsorbate—metal surface systems in which structures incommensurate with the substrate are observed is extremely large. Among them can be distinguished an entire class of systems in which the incommensurate structure is produced through the compression of the commensurate structure along one of the crystallographic directions of the substrate.[3-6] Such incommensurate structures can be described with the aid of a simple model of a two-dimensional anisotropic crystal in which only the adatom displacements along the direction of the compression are considered.

The behavior of such a model has been theoretically studied in various papers,[7-11] starting from Frank and Van der Merwe's classic paper.[7] It has been established that a periodic lattice of solitons—compression or extension regions compensating for the difference between the lattice constants of the film and the substrate—occur in the ground state of such an incommensurate crystal in the vicinity of the commensurability point. It is precisely this lattice that is responsible for the acoustic branch in the excitation spectrum. Outside the solitons the adatoms reside at the minima of the potential relief. Therefore, the properties of the incommensurate crystal near the commensurability point are in fact determined by the behavior of the soliton lattice. The properties of such a lattice are studied in the present paper. To do this, we systematically reduce the problem of the soliton lattice of an incommensurate anisotropic crystal to the problem of the XY model, whose properties have been studied in detail. It is shown that, in the long-wave limit, the Hamiltonian and the correlation function of the incommensurate crystal can be expressed in terms of the Hamiltonian and the correlation function of the XY model. The direct interaction between the solitons (because of their slight overlap) decreases exponentially with distance. But the interaction via the elastic deformations of the substrate decreases according to a power law, and is substantial in the case of large lattice constants. Therefore, below we solve the problem of the incommensurate crystal on an elastic substrate self-consistently.

It is significant that the energy of the interaction of the solitons via the substrate is determined not by the small amplitude of the potential relief of the substrate, but by the ratio of the elastic moduli of the film and the substrate, which ratio is not particularly small. One of the consequences of the interaction via the elastic deformations of the substrate is the alteration of the phase diagram. The question of the phase diagram is considered in Refs. 12–14. It is shown[12,13] that, when the degree of commensurability is equal to, say, unity, the melting point of the soliton lattice tends to zero as the commensurability point is approached. But the melting point does not decrease at higher degrees of commensurability.[13] In the present paper we show that, even when the degree of commensurability is equal to unity, the melting point has a finite minimum because of the interaction via the elastic modes of the substrate. The results obtained in the present paper allow us to predict, besides the phase diagram, the dependence of the superstructure reflections of the soliton lattice on the temperature and the coverage. Some of the results obtained below (the dislocation mechanism of soliton-lattice melting) were published earlier.[12]

2. CONSTRUCTION OF THE MODEL

As a rule, two-dimensional anisotropic incommensurate crystals are formed on faces with a fluted potential relief of the W(112) type, but there are examples of such systems on faces with a relatively isotropic relief, e.g., CO–Pt(111), CO–Ni(111), and CO–Pd(111) (Ref. 4). The majority of the available systems are chemisorbed adfilms, but there is also an example of physisorbed systems: Xe–Cu(110) (Ref. 6). In the case of chemisorption on faceted faces,[3,5] the incommensurate structures are formed because of the presence of

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strong repulsion due, for example, to the presence of a large dipole moment. As adsorbates we can use alkali (Li, Na, K, Cs), alkaline-earth (Sr, Ba), and rare-earth (La) elements; as substrates, the faces W(112), Mo(112), Re(10$\bar{1}$0), and Ni(110). The symmetries of these structures may be different: e.g., the unit cell may be centered [K–W(112) (Ref. 5)], primitive [Li–W(112) (Ref. 5)], or of a more complex structure [Na–Ni(110) (Ref. 3)].

For the purposes of the present paper (the investigation of the general properties of the soliton lattice), it is convenient to consider the simplest case of a rectangular primitive unit cell near the point at which the fundamental lattice constants of the film and the substrate are equal. The contraction (or extension) of such a structure as the coverage is increased (decreased) occurs along the troughs of the potential relief. Two-dimensional anisotropic crystals can be described by a model in which only the displacements along the direction of the contraction are considered. In the case of a primitive unit cell the elastic Hamiltonian of such a model without allowance for the potential of the substrate has the form

$$H=\frac{1}{2}\int dxdy\left\{\lambda_1\left(\frac{\partial w}{\partial x}\right)^2+\lambda_2\left(\frac{\partial w}{\partial y}\right)^2\right\}, \tag{1}$$

where λ_1 and λ_2 are the elastic moduli and w is the displacement along the direction of the contraction of the structure. A term of the type $(\partial w/\partial x)(\partial w/\partial y)$ is forbidden by the symmetry of a structure with a primitive unit cell. Allowance for such a term can (under certain conditions) only lead to the inclination of the soliton lattice, and does not alter the results of the present paper. We shall assume that the potential $\mu(x)$ of the interaction with the substrate (the modulation of the potential relief along the troughs) is much smaller than the interadatom interaction energy. The strong inequality may not be satisfied in an actual experimental situation, but the qualitative picture should not change if the incommensurate phase indeed exists. As indicated above, the problem can be simplified further by considering the situation in which the lattice constants, a and b, of the film and the substrate are nearly equal to each other. The results can easily be generalized to the case of arbitrary degrees of commensurability, i.e., of arbitrary values of $a/b=m/n$.

The Hamiltonian of the described model and the properties of the ground state have been well known since the publication of Frank and Van der Merwe's paper.[7] Therefore, we shall only write down the Hamiltonian and the ground state. The Hamiltonian itself has the form

$$H=\int dxdy\left\{\frac{1}{2}\lambda_1\left(\frac{\partial w}{\partial x}\right)^2+\frac{1}{2}\lambda_2\left(\frac{\partial w}{\partial y}\right)^2+\mu[wq_0+(k_0-q_0)x]\right\}, \tag{2}$$

or, in dimensionless variables, the form

$$H=\frac{(\lambda_1\lambda_2)^{1/2}}{q_0^2}\int dsdt\left\{\frac{1}{2}\left(\frac{\partial\varphi}{\partial s}-p\right)^2+\frac{1}{2}\left(\frac{\partial\varphi}{\partial t}\right)^2+f(\varphi)\right\}. \tag{3}$$

Here we have made the following change of variables: for the potential of the substrate $\mu(\varphi)=\mu_0 f(\varphi)$, where $\mu_0=|\min f(\varphi)|$, $f(\varphi)\geq -1$; for the coordinates x and y

$$x=s(\lambda_1/\mu_0)^{1/2}q_0^{-1},\quad y=t(\lambda_2/\mu_0)^{1/2}q_0^{-1};$$

and for the displacement

$$w=(\varphi-ps)q_0^{-1},\quad p=(k_0-q_0)q_0^{-1}(\lambda_1/\mu_0)^{1/2},\quad k_0=2\pi/b,\quad q_0=2\pi/a.$$

To find the ground state of the Hamiltonian (3), we must vary (3) with respect to φ, which leads to the equation

$$\partial^2\varphi/\partial s^2+\partial^2\varphi/\partial t^2-\dot{f}(\varphi)=0. \tag{4}$$

Here the dot denotes differentiation with respect to φ. We shall seek the ground state as a function of only s. The method of obtaining the solution is described in detail in Pokrovskiĭ and Talapov's paper.[1] The solution (i.e., the ground state) $\varphi_0(s)$ is given by the integral:

$$s+s_0=\int_0^{\varphi_0}\frac{d\varphi}{[2(\varepsilon+f(\varphi))]^{1/2}}. \tag{5}$$

The energy density is given by the expression

$$U=\frac{1}{q_0^2}(\lambda_1\lambda_2)^{1/2}\left\{\frac{I_1(\varepsilon)}{I_2(\varepsilon)}-\varepsilon+\frac{1}{2}p^2\right\}, \tag{6}$$

where $I_1(\varepsilon)$ and $I_2(\varepsilon)$ are defined by analogy with the complete elliptic integrals:

$$I_1(\varepsilon)=\int_0^{2\pi}[2(\varepsilon+f(\varphi))]^{1/2}d\varphi,\quad I_2(\varepsilon)=\int_0^{2\pi}\frac{d\varphi}{[2(\varepsilon+f(\varphi))]^{1/2}}. \tag{7}$$

Normally, the quantity ε (see Ref. 1) is found from the condition for the energy to be a minimum. This corresponds to a system in which the chemical potential (the pressure of the gaseous adsorbate) is prescribed. This situation is realized in the case in which an inert gas is adsorbed on graphite. In the case of metal adfilms the lattice constant of the substrate is strictly prescribed by the deposition conditions. Therefore, in this case the quantity ε is determined from the condition

$$I_2(\varepsilon)=2\pi/p. \tag{8}$$

The solution (5)–(8) describes a periodic superlattice formed by the adatoms. Over the period l of this lattice ($l=2\pi/p$) the function φ_0 changes by 2π. This change is concentrated in a region (i.e., in a soliton) of dimension l_0 [$l_0\sim 1$ in the measurement units used in (4)]. Outside the soliton the change in φ_0 is exponentially small. The most important property of the solution (5)–(8) is the presence of a continuous translation group. This allows us (when $l>l_0$) to speak of a soliton lattice and its elastic properties. The intersoliton interaction energy decreases exponentially with increasing l in the solution (5)–(8). But it turns out that there also exists a power contribution to the soliton repulsion energy. Although this contribution is small compared to the characteristic energy of a soliton, it is decisive in the case of large soliton-lattice constants. One of the causes of the power-law decrease of the intersoliton interaction energy is the deformation of the substrate.

3. THE ELASTIC SUBSTRATE

The adatoms undergo displacements from the minima of the potential relief during the formation of the soliton, and this leads to the deformation of the elastic substrate. These deformations decrease according to

a power law, and guarantee the power-law weakening of the interaction between the solitons.[15] To carry out an accurate analysis of this intersoliton interaction mechanism, we must solve the self-consistent problem of the incommensurate crystal on an elastic substrate. For simplicity of analysis, we shall assume that the substrate is elastically isotropic. Furthermore, we shall assume that the substrate is significantly more rigid than the adfilm (the criterion will be derived below), which corresponds to the experimental situation for adatoms on metallic substrates. In this case the substrate deformations will be considerably smaller than the adfilm deformations, and the interaction between the film and the substrate can be taken into account by considering in the film–substrate interaction energy the displacement $w' = w - u_x$ (where u_x is the deformation of the substrate along the x axis) instead of the displacements w. As a result, the Hamiltonian of the adfilm will have the form

$$H = \int dxdy \left\{ \frac{1}{2}\lambda_1 \left(\frac{\partial w}{\partial x}\right)^2 + \frac{1}{2}\lambda_2 \left(\frac{\partial w}{\partial y}\right)^2 + \mu_0 f(q_0(w-u_x) + (k_0 - q_0)x) \right\}. \tag{9}$$

Since in the system under consideration the solitons are oriented along the y axis, it is sufficient to consider only the substrate deformations in the xz plane. To the surface of the crystal corresponds $z = 0$; to the substrate, $z > 0$. Then the Hamiltonian for the elastic deformations of the substrate can be written in the form[16]

$$H_s = \frac{1}{2}\int dxdy \int_0^\infty dz \{\sigma_{xx}u_{xx} + \sigma_{zz}u_{zz} + 2\sigma_{xz}u_{xz}\}, \tag{10}$$

where the σ_{ik} are the elements of the stress tensor and the u_{ik} are the elements of the strain tensor. To find the elastic-deformation energy of the substrate for a given $u_x(x)$, we must solve the equations of the two-dimensional elasticity theory with the boundary conditions $u_{xx}(x, 0) = \partial u_x/\partial x$, $u_{xz}(x, 0) = 0$. The corresponding equations have the form[16]

$$\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xz}}{\partial z} = 0, \quad \frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{zz}}{\partial z} = 0. \tag{11}$$

The solution to these equations has (in the Fourier representation with respect to the x coordinate) the following form:

$$\begin{aligned} \sigma_{xx}(q, z) &= \frac{E}{1-\sigma} u_{xx}(q, 0)(1 + |q|z)e^{-|q|z}, \\ \sigma_{zz}(q, z) &= \frac{E}{1-\sigma} u_{xx}(q, 0)(1 - |q|z)e^{-|q|z}, \\ \sigma_{xz}(q, z) &= \frac{E}{1-\sigma} iqz u_{xx}(q, 0)e^{-|q|z}. \end{aligned} \tag{12}$$

Here E is Young's modulus and σ is the Poisson coefficient. Substituting the solution (12) into (10), and performing the integration over z, we easily obtain an expression for the elastic-substrate-deformation Hamiltonian as a function of the adfilm-induced deformations of the substrate:

$$H_s = \frac{E}{(1-\sigma)^2}\int dydq |u_{xx}(q)|^2/|q|. \tag{13}$$

Making the substitution $\psi = q_0(w - u_x) + (k_0 - q_0)x$ in (9), and minimizing the elastic energy at a fixed value of ψ, we easily obtain an expression for the Hamiltonian of an adfilm on an elastic substrate:

$$H = \int dxdy \left\{ \frac{1}{2}\lambda_1' q_0^{-2} \left(\frac{\partial \psi}{\partial x} - p'\right)^2 + \frac{1}{2}\lambda_2 \left(\frac{\partial \psi}{\partial y}\right)^2 q_0^{-2} + \mu_0 f(\psi) + \int dx' \left(q_0^{-2} \frac{\partial \psi}{\partial x} \frac{\partial \psi}{\partial x'} g(x - x') \right) \right\}, \tag{14}$$

where

$$\begin{aligned} \frac{1}{\lambda_1'} &= \frac{1}{\lambda_1} + \frac{1}{\lambda_0}, \quad p' = \frac{\lambda_1}{\lambda_1'}(k_0 - q_0), \quad \lambda_0 = \frac{2Eq_0^{-1}}{(1-\sigma)^2} \\ g(x - x') &= \lambda_1' \frac{\lambda_1}{2\lambda_0 q_0} \frac{1}{(x - x')^2}. \end{aligned} \tag{15}$$

Here λ_0 is the effective contribution to the rigidity of the adfilm as a result of the elastic deformations of the substrate. The requirement that the substrate be rigid implies that $\lambda_0 \gg \lambda_1$. An important characteristic of the expression obtained is the renormalization of the parameters of the adfilm's Hamiltonian [besides the appearance of a nonlocal substrate-mediated interaction (see also Ref. 17)]. This is the difference between the above-obtained solution and the solution given in Ref. 15. In contrast to the results obtained in Ref. 15, the above-presented self-consistent solution allows only soliton repulsion (in the case of an elastically isotropic substrate). The quantity $\partial\psi/\partial x$ is nonzero only in the region of the soliton; outside the soliton ψ varies exponentially slowly. Therefore, in the first approximation in λ_1/λ_0 the contribution to the energy density from the substrate-mediated interaction can be taken into account by substituting the solution φ_0 (with the renormalized constants λ_1' and p') in place of ψ.

In the case in which $l \gg l_0$, we can replace the integration in (14) over the entire x and x' by integration over the lattice constant and summation over the solitons. As a result, we easily obtain the contribution to the energy density from the interaction of the solitons:

$$E_s = \frac{1}{12}\frac{a^3}{l^3}\lambda_1' \frac{\lambda_1}{\lambda_0}. \tag{16}$$

The power-law character of the dependence (16) and, what is more, the magnitude of the exponent play an important role in the thermodynamics of the soliton lattice. It should be noted that the interaction mediated by the elastic modes of the substrate is the only interaction between the solitons that falls off at $T = 0$ according to a power law. The presence of long-range interactions (i.e., interactions that fall off according to a power law) between the adatoms does not change this assertion, since this circumstance in no way manifests itself in the calculations performed on the basis of the theory of elasticity. At $T \neq 0$ there is another reason for the appearance in the energy density of a contribution that is a power function of l: the collisions between the solitons. The magnitude of the contribution of this nonlinear process is computed in Ref. 1, and is equal to

$$E_t = \pi^2 T^2/6l^3\varepsilon_0, \tag{17}$$

where ε_0 is the density of the energy in the soliton: $\varepsilon_0 \sim (\lambda_1\mu_0)^{1/2}a$.

4. THE SOLITON LATTICE IN THE XY MODEL

The soliton–soliton interaction energy decreases as the soliton spacing increases. On the other hand, the energy connected with the destruction of the soliton itself is not small, and does not decrease with increasing l. As follows from the Hamiltonian (3), this is, in order of magnitude, equal to

$$q_0^{-2}(\lambda_1\lambda_2)^{1/2}l_0^2 \sim q_0^{-2}(\lambda_1\lambda_2)^{1/2}.$$

Thus, we can, in the case of excitation energies much lower than $q_0^{-2}(\lambda_1\lambda_2)^{1/2}$, consider only the elastic deformations of the soliton lattice (flexure, compression). To describe such long-wave excitations, it is convenient to use the effective Hamiltonian for the soliton-lattice displacements, which is obtainable from the Hamiltonian (3) through averaging over the period of the soliton superlattice. The elastic moduli of the soliton lattice is most simply obtained by averaging Eq. (4) for the case of deformations with a long wavelength over the period of the soliton structure. For this purpose, we use a perturbation-theory expansion similar to the one used in Ref. 1 to determine the spectrum of the small vibrations. If $\varphi_0(s)$ [see (5)–(8)] is the ground state of the Hamiltonian (3), then $\varphi_0(s+u)$, where $u=\text{const}$, is the solution describing the displacement of the entire soliton lattice through a distance u. We shall seek the solution $\varphi(s+u)$ for the inhomogeneous deformation in the form of an expansion in powers of the derivatives of u. Then in the first approximation

$$\varphi(s+u)=\varphi_0(s+u)+\frac{\partial u}{\partial s}\varphi_1(s+u). \tag{18}$$

Substituting (18) into (4), we obtain for $\varphi_1(s+u)$ from the requirement that (4) be fulfilled in first order in $\partial u/\partial s$ the equation (a prime denotes differentiation with respect to s):

$$\varphi_1''-(\varphi_0'''/\varphi_0')\varphi_1+2\varphi_0''=0. \tag{19}$$

The solution to Eq. (19), that is periodic in s with period l, has the form

$$\varphi_1(s)=\varphi_0'(s)\left(\int_0^s\frac{dz}{(\varphi_0'(z))^2}-s\right)\Big/\int_0^l\frac{dz}{(\varphi_0'(z))^2}. \tag{20}$$

In the next order in the derivatives, we have

$$\varphi(s+u)=\varphi_0(s+u)+\frac{\partial u}{\partial s}\varphi_1(s+u)+\frac{\partial^2 u}{\partial s^2}\varphi_2(s+u). \tag{21}$$

The t derivatives in this order should not be included in the expansion yet. Substituting (21) into (4), and making allowance for (19), we obtain the equation

$$\left(\varphi_0'+2\varphi_1'+\varphi_2''-\frac{\varphi_0'''}{\varphi_0'}\varphi_2\right)\frac{\partial^2 u}{\partial s^2}+\varphi_0'\frac{\partial^2 u}{\partial t^2}=0. \tag{22}$$

Multiplying it by φ_0', and averaging over the soliton-lattice constant (with allowance for the periodicity of φ_0 and φ_2), we obtain the following equations:

$$\tilde\Lambda_1\frac{\partial^2 u}{\partial s^2}+\tilde\Lambda_2\frac{\partial^2 u}{\partial t^2}=0,$$
$$\tilde\Lambda_1^{-1}=\int_0^l\frac{dx}{(\varphi_0'(x))^2}=-\frac{dI_2}{d\varepsilon},\quad \tilde\Lambda_2=\frac{1}{l}\int_0^l(\varphi_0'(x))^2dx=\frac{I_1(\varepsilon)}{I_2(\varepsilon)}. \tag{23}$$

A similar computational procedure allows us to obtain the elastic-deformation Hamiltonian of the soliton lattice:

$$H_s=\frac{(\lambda_1\lambda_2)^{1/2}}{q_0^2}\int ds\,dt\left\{\frac{1}{2}\tilde\Lambda_1\left(\frac{\partial u}{\partial s}\right)^2+\frac{1}{2}\tilde\Lambda_2\left(\frac{\partial u}{\partial t}\right)^2\right\}. \tag{24}$$

In the original coordinates x and y, we have

$$H_s=\int dx\,dy\left\{\frac{1}{2}\Lambda_1\left(\frac{\partial v}{\partial x}\right)^2+\frac{1}{2}\Lambda_2\left(\frac{\partial v}{\partial y}\right)^2\right\}, \tag{25}$$

where $v=u(\mu_0/\lambda_1)^{1/2}q_0^{-1}$ is the soliton displacement expressed in terms of the original coordinates,

$$\Lambda_1=\mu_0\tilde\Lambda_1,\quad \Lambda_2=(\lambda_2/\lambda_1)\mu_0\tilde\Lambda_2.$$

The behavior of Λ_1 and Λ_2 at large l can be represented as follows:

$$\Lambda_1=A\frac{\varepsilon_0}{l}e^{-l/l_0},\quad \Lambda_2=\frac{\varepsilon_0}{l}, \tag{26}$$

where A is a numerical constant depending on the details of the potential $f(\varphi)$.

The obtained Hamiltonian is isomorphic to the Hamiltonian of the XY model.[18-20] Let us consider how the adatom-displacement correlation function $G(\mathbf{R}-\mathbf{R}')$ can be expressed in terms of the correlation function of the XY model. By definition, we have

$$\begin{aligned}G(\mathbf{R}-\mathbf{R}')&=\langle\rho_0^2\exp[iq_0(x+w(\mathbf{R})-x'-w(\mathbf{R}'))]\rangle\\&=\rho_0^2\exp(ik_0(x-x'))\langle\exp[i(\varphi(\mathbf{R})-\varphi(\mathbf{R}'))]\rangle.\end{aligned} \tag{27}$$

Here $\mathbf{R}=(x,y)$, ρ_0 is the amplitude of the density wave, and the brackets $\langle\ldots\rangle$ denote averaging over the states of the Hamiltonian (3). We shall be interested in the asymptotic form of $G(\mathbf{R}-\mathbf{R}')$ at distances much greater than the soliton-lattice constant. Then the function $\varphi(\mathbf{R})$ can be represented in the form $\varphi(\mathbf{R})=\varphi_0[s+u(s,t)]$. The function $\exp[i\varphi_0(s)]$ can be expanded in a Fourier series, since $\varphi_0(s)$ is a periodic function with period l. We can, in investigating the asymptotic form of the correlator (27), limit ourselves to the first harmonic. As a result, we obtain

$$G(\mathbf{R}-\mathbf{R}')=\rho_0^2e^{ik_0(x-x')}\frac{1}{l^2}\left|\int_0^l\exp\left[i\varphi_0(x)+2\pi i\frac{x}{l}\right]dx\right|^2G_s(\mathbf{R}-\mathbf{R}'), \tag{28}$$

$$G_s(\mathbf{R}-\mathbf{R}')=\left\langle\exp\left[i\frac{2\pi}{l}(v(\mathbf{R})-v(\mathbf{R}'))\right]\right\rangle_s. \tag{29}$$

Here G_s is the correlation function in the XY model and the subscript s attached to the brackets indicates that the averaging is performed over the states of the Hamiltonian H_s, (25), of the soliton lattice. Notice that the expression (29) for the correlator does not go over into the correlator in the commensurate structure when we go to the limit $l\to\infty$, since it is derived under the assumption that the distances are much greater than the soliton-lattice constant. The above-presented results show that, in the long-wave asymptotic form, the problem of the two-dimensional incommensurate anisotropic crystal in the vicinity of the commensurability point reduces to the problem of the XY model.

The behavior of the XY model is decisively affected by the topologically stable defects: the vortices. In the present system they correspond to dislocations in the

soliton lattice. Let us consider how these dislocations are formed.

The character of defects in systems with a continuous symmetry group depends, in the presence of perturbations that break this symmetry, on the dimensions of the region under consideration.[21,22] The problem contains three characteristic lengths: the interatomic distance a, the soliton width l_0, and the soliton spacing l; the quantity l_0 also determines the scale of the localization of the perturbations in the adatom lattice. Therefore, a dislocation in the adatom lattice in the region of distances $a < r < l_0$ will change into a soliton with the end at the center of the dislocation for distances $l_0 < r < l$. Such a soliton with the end in the region of distances $r > l$ can be regarded as a dislocation in the soliton lattice. In this region of distances we can write the solution in the form (18), in which we must substitute for the displacement v the standard solution for a dislocation:

$$v = l \operatorname{arctg}\left[\frac{x}{y}\left(\frac{\Lambda_2}{\Lambda_1}\right)^{1/2}\right]. \tag{30}$$

Here the lattice constant l plays the role of the Burgers dislocation vector. In the case of a degree of commensurability $a/b = m/n$ one extra row of adatoms is equivalent to m solitons. Therefore, the smallest Burgers vector will be equal to ml. This circumstance plays an important role in the estimation of the contribution of the dislocations to the thermodynamics of the system.

5. MELTING AND DIFFRACTION REFLECTIONS

The conclusion that the soliton lattice and the XY model are isomorphic was drawn above without allowance for the mechanism underlying the long-range repulsion (16) and (17). But the isomorphism should remain if the change that occurs in the compression modulus Λ_1 as a result of the presence of the interactions (16) and (17) is taken into account. Therefore, the mechanism underlying the melting of the soliton lattice should also be similar to the underlying phase transition in the XY model.

The mechanism underlying the phase transition in the XY model is connected with the behavior of the vortices.[18-20] Below the transition temperature the vortices form bound pairs; above this temperature these pairs break up into separate vortices. In the process the power-law decrease of the correlators, which is characteristic of the ordered phase in the XY model, is replaced by an exponential decrease in the high-temperature phase. Therefore, in the case of the soliton lattice the phase transition (the vanishing of the elastic moduli at large distances) will occur at the point where the dislocation pairs break up into individual dislocations. The corresponding temperature T_p will be given by the expression for the transition temperature for the XY model:

$$T_p = (\Lambda_1\Lambda_2)^{1/2} m^2 l^2/8\pi. \tag{31}$$

The additional contribution to the compression modulus from the terms in the energy density (16) and (17) can be computed by using the fact that the compression modulus

$$\Lambda_1 = l^2 \partial^2 E/\partial l^2. \tag{32}$$

As a result, for Λ_1 and Λ_2 we have:

$$\Lambda_1 = A\frac{\varepsilon_0}{l}e^{-l/l_0} + \frac{1}{l^2}\left(\lambda_1' a^3 \frac{\lambda_1}{2\lambda_0} + \frac{\pi^2 T^2}{\varepsilon_0}\right), \quad \Lambda_2 = \frac{\varepsilon_0}{l}. \tag{33}$$

Substituting (33) into (31), we obtain an expression for the melting point:

$$T_p = \frac{1}{\pi(64/m^2-1)^{1/2}}\left\{A\varepsilon_0^2 \frac{l^4}{l_0^2}e^{-l/l_0} + \frac{\varepsilon_0}{2}\lambda_1' a^3 \frac{\lambda_1}{\lambda_0}\right\}^{1/2}. \tag{34}$$

If $m^2 > 64$, then the expression (34) is meaningless. This means that, for large m, the soliton lattice is stable against the production of dislocations because of their long Burgers vector and the presence of an entropy-governed repulsion.[13] If $m = 1, 2$, then the melting temperature has a minimum in the vicinity of the commensurability point ($l \to \infty$), but it does not vanish either. This is prevented by the presence of the interaction mediated by the elastic modes of the substrate. The minimum value T_{min} of the melting temperature is given by the following expression:

$$T_{min} = \frac{1}{\pi(64/m^2-1)^{1/2}}\left(\varepsilon_0\lambda_1' a^3 \frac{\lambda_1}{2\lambda_0}\right)^{1/2}. \tag{35}$$

Thus, if the ratios μ_0/λ_1 and λ_1/λ_0 are not too small, then T_{min} can be fairly high. In the considered case of metal-film systems the dependence $T_p(l)$ automatically gives the dependence of T_p on the coverage Θ, since $l \sim |\Theta - \Theta_0|^{-1}$, where Θ_0 is the coverage of the commensurate structure. For example, in the case in which the degree of commensurability is equal to unity $l = a|1-\Theta|^{-1}$.

The above-presented results allow us to compute the dependence of the intensity of the superstructure reflections of the soliton lattice on the temperature and the coverage. The general form of the diffraction pattern in the incommensurate phase is derived in Ref. 1. In the vicinity of the point where the degree of commensurability is equal to unity (i.e., where $a/b = 1$), the diffraction pattern consists of a central peak at $q_0 = k_0$, which corresponds to the commensurable structure, and satellites at $q = k_0 \pm 2\pi/l$, where $2\pi/l$ is the reciprocal lattice vector of the soliton structure. At low temperatures, i.e., at temperatures lower than T_p, the decrease of the intensity I of the superstructure reflections with temperature will be described by the Debye-Waller factor W:

$$I \sim \left|\frac{1}{l}\int_0^l \exp\left\{i\varphi_0(x) + 2\pi i\frac{x}{l}\right\}dx\right|^2 e^{-2W}, \tag{36}$$

$$W = \frac{\pi T}{l^2(\Lambda_1\Lambda_2)^{1/2}}\ln Rq_0. \tag{37}$$

Here R is the characteristic (minimum) dimension of the system. The first factor in (36) is simply the soliton density, which tends to zero as the commensurability point is approached. The behavior of the second factor in the vicinity of the commensurability point is determined by the quantity $l^2(\Lambda_1\Lambda_2)^{1/2}$. Using the expressions (33) for Λ_1 and Λ_2, we obtain for W for $l \to \infty$ the expression

$$W=T\left\{\frac{e_0\lambda_1'a^3\lambda_1}{2\pi^2\lambda_0}+T^2\right\}^{-1/2}\ln Rq_0. \tag{38}$$

Thus, W has a finite limit at the commensurability point.

Let us consider the experimental consequences of the results obtained. The first of them is the possibility of observing a minimum in the melting temperature of the soliton lattice at the commensurability point. The second is the behavior, described by the formulas (36)–(37), of the intensity of the superstructure reflections at low temperatures. The experimental characteristic determining the feasibility of the observation of the indicated phenomena is the limited resolving power of the apparatus (i.e., the coherence length). In the case of the LEED method this quantity ~100 Å. The above-presented results (e.g., for T_p) were obtained for an unbounded system, or, more exactly, for a system in which the distances between the dislocation pairs are significantly smaller than its dimension. Therefore, the melting point was found not to depend on the dislocation concentration. But the energy of the dislocation center is high: of the order of the interadatom interaction energy. Therefore, the distances between the pairs can be greater than the coherence length even at T_p. Therefore, the smearing of the superstructure reflections can occur at temperatures significantly higher than the T_p, (34), for an unbounded system.

The quantity I, (36), should go to zero near the commensurability point like l^{-2}. Therefore, as a function of the coverage Θ,

$$I\sim(\Theta-\Theta_0)^2. \tag{39}$$

In a real situation the dependence (39) will be smeared out by the concentration fluctuations in a region of dimension of the order of the coherence length. As a result, the intensity I will simply have a minimum, and not vanish, at $\Theta=\Theta_0$.

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[1]V. L. Pokrovskiĭ and A. L. Talapov, Zh. Eksp. Teor. Fiz. **78**, 269 (1980) [Sov. Phys. JETP **51**, 134 (1980)].
[2]A. G. Naumovets and A. G. Fedorus, Zh. Eksp. Teor. Fiz. **73**, 1085 (1977) [Sov. Phys. JETP **46**, 575 (1977)].
[3]R. L. Gerlach and T. N. Rhodin, Surf. Sci. **17**, 32 (1969).
[4]G. Ertl and J. Koch, Z. Naturforsch. Teil A **25**, 1306 (1970); K. Christmann, O. Schober, and G. Ertl, J. Chem. Phys. **60**, 4719 (1974); G. Ertl, M. Neumann, and K. M. Streit, Surf. Sci. **64**, 393 (1977).
[5]J. M. Chen and C. A. Papogeorgopoulos, J. Vac. Sci. Technol. **9**, 570 (1972); V. K. Medvedev and T. P. Smereka, Fiz. Tverd. Tela (Leningrad) **15**, 724 (1973) [Sov. Phys. Solid State **15**, 507 (1973)]; V. K. Medvedev and A. I. Yakivchuk, Fiz. Tverd. Tela (Leningrad) **16**, 981 (1974) [Sov. Phys. Solid State **16**, 634 (1974)]; V. K. Medvedev and A. I. Yakivchuk, Ukr. Fiz. Zh. **20**, 1900 (1975); Yu. S. Vedula, V. K. Medvedev, A. G. Naumovets, and V. N. Pogorelyĭ, Ukr. Fiz. Zh. **22**, 1826 (1977); V. K. Medvedev and I. N. Yakovkin, Fiz. Tverd. Tela (Leningrad) **23**, 669 (1981) [Sov. Phys. Solid State **23**, 379 (1981)]; M. S. Gupalo, Fiz. Tverd. Tela (Leningrad) **22**, 2311 (1980) [Sov. Phys. Solid State **22**, 1345 (1980)].
[6]M. Jaubert, A. Glachaut, M. Bienfait, and G. Boato, Phys. Rev. Lett. **46**, 1679 (1981).
[7]F. C. Frank and J. H. Van der Merwe, Proc. R. Soc. London **198**, 205 (1949).
[8]A. Luther, J. Timonen, and V. Pokrovsky, Nordita Preprint 79/30, 1979.
[9]Y. Okwamoto, J. Phys. Soc. Jpn. **49**, 1 (1980).
[10]H. J. Shulz, Phys. Rev. B **22**, 74 (1980).
[11]F. D. M. Haldane and J. Villain, Preprint, 1980.
[12]I. F. Lyuksyutov, Pis'ma Zh. Eksp. Teor. Fiz. **32**, 593 (1980) [JETP Lett. **32**, 579 (1980)].
[13]S. N. Coppersmith, D. S. Fisher, B. I. Halperin, P. A. Lee, and W. F. Brinkman, Phys. Rev. Lett. **46**, 549 (1981).
[14]I. Lyuksyutov and V. L. Pokrovsky, J. Phys. Lett. (Paris) **43**, L-11 (1982).
[15]M. B. Gordon and J. Villain, J. Phys. C **12**, L151 (1979).
[16]L. D. Landau and E. M. Lifshitz, Teoriya uprugosti (Theory of Elasticity), Nauka, Moscow, 1965 (Eng. Transl., Pergamon, Oxford, 1970).
[17]L. A. Bol'shov, M. S. Veshchunov, and A. M. Dykhne, Zh. Eksp. Teor. Fiz. **80**, 1997 (1981) [Sov. Phys. JETP **53**, 1038 (1981)].
[18]V. L. Berezinskiĭ, Zh. Eksp. Teor. Fiz. **59**, 907 (1970) [Sov. Phys. JETP **32**, 493 (1971)].
[19]J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973).
[20]J. V. Jose, L. P. Kadanoff, S. Kirkpatrick, and D. Nelson, Phys. Rev. B **16**, 1217 (1977).
[21]G. E. Volovik and V. P. Mineev, Zh. Eksp. Teor. Fiz. **72**, 2256 (1977) [Sov. Phys. JETP **45**, 1186 (1977)].
[22]V. P. Myneyev and G. E. Volovik, Phys. Rev. B **18**, 3197 (1978).

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