Multicritical point of a two-dimensional incommensurable crystal

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The melting of a soliton superstructure of an adfilm near the commensurability point is investigated. It is shown that the bulk modulus of a soliton lattice vanishes at this point. A mechanism for formation of dislocations is determined. A phase diagram, in which the commensurability point is a multicritical point, is obtained.

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Two-dimensional structures, which have an incommensurable lattice with a substrate, have been observed in a large number of adsorbate-substrate systems. These are, for example, graphite-based, noble gas films[1] and films of alkali atoms and alkali-earth atoms on refractory metal substrates.[2] An incommensurable structure in metallic substrates can be formed by compressing a commensurable structure in certain crystallographic directions of the substrate, which are determined by the anisotropy of the charge image. In constructing a model of a phase transition from a commensurable phase to an incommensurable phase, it is sufficient to consider the displacement of adatoms only in the direction of compression. Another simplification involves the use of an adatom lattice with a primitive cell [experimental examples are Li-W(112) and Li-Mo (112) (Ref. 3)].

The model Hamiltonian can be written in the form (for details, see Ref. 4)

$$H = \int dxdy\left\{ \frac{1}{2}\lambda_1\left(\frac{\partial u}{\partial x}\right)^2 + \frac{1}{2}\lambda_2\left(\frac{\partial u}{\partial y}\right)^2 + v\cos\phi \right\}. \tag{1}$$

Here $u(x,y)$ is the lattice displacement, λ_1 and λ_2 are the elastic constants of the adfilm, v is the amplitude of the substrate's charge image, $\phi = 2\pi b^{-1}\ [u + (a-b)a^{-1}\ x]$, and a and b are adjacent periods of the film and of the substrate. The Hamiltonian (1) corresponds to a lattice with free ends. Since the interaction of alkali adatoms is repulsive,[3] they can be described by the "compressed"-lattice model in which the period of the film is determined by the concentration c of the adatoms. This can be formally accomplished by introducing an appropriate Lagrangian multiplier μ and by introducing the term $\mu[\partial\phi/\partial x - 2\pi b^{-1}(1-c)]$ in Eq. (1).

A superstructure lattice of linear solitons with a one-dimensional periodicity appears in an incommensurable phase near the commensurability point ($a/b \sim 1$). The transverse dimension of a soliton is $l \sim b\lambda_1^{1/2}\ v^{-1/2}$, the displacement u due to soliton motion varies by the amount of the lattice spacing, and the phase ϕ varies by 2π. After the displacement u decreases exponentially at the soliton boundary. The distance between the solitons L is determined by the ratio a/b. The period L approaches infinity at the commensurable-incommensurable phase transition point. The soliton superstructure has a continuous translation group relative to the substrate.[4] At sufficiently low temperatures $T \ll v, \lambda_1$, and λ_2, we can regard it as a new, two-dimensional lattice on a smooth substrate.

We investigate in this paper the melting of such a lattice near the commensurability point. To do this, we must calculate the elastic moduli of the soliton lattice and determine the mechanism for formation of dislocations in it. The energy variation $\delta\varepsilon$ due to convergence δu of two solitons of length L is $\delta\varepsilon \sim \lambda_1 L^2 l^{-2} \exp(-Ll^{-1})$ $(\delta u)^2$. Therefore, the bulk modulus of a soliton lattice is $\Lambda_1 \sim \lambda_1 L^2 l^{-2} \exp(-Ll^{-1})$. As follows from Eq. (1), the shear modulus Λ_2 cannot vary as a result of variation of the dimensions; therefore, $\Lambda_2 \sim \lambda_2$. Thus, the soliton lattice can be described by means of the Hamiltonian

$$H = b^2(2\pi)^{-2}(\Lambda_1\Lambda_2)^{1/2} \int ds\, dt \left\{ \frac{1}{2}\left(\frac{\partial \phi}{\partial s}\right)^2 + \frac{1}{2}\left(\frac{\partial \phi}{\partial t}\right)^2 \right\}. \tag{2}$$

Here $s = x\Lambda_1^{-1/2}$, $t = y\Lambda_2^{-1/2}$. The mechanism for melting of a two-dimensional crystal is associated with the interaction of dislocations.[5] The dislocations are bound in pairs below the transition point and are free above it.

We shall examine the mechanism for formation of dislocations in a soliton lattice. Suppose a dislocation is formed in the adatom lattice. It can be represented, for example, as an excessive series of atoms, which is cut off in the dislocation center. By tracing an arbitrary path around such a center, we can see that the phase advance ϕ is equal to 2π. Since the adatom lattice is located on the substrate, its deformations must be localized at a distance of the order of $l_0 \sim bv^{-1/2}\max(\lambda_1^{1/2}, \lambda_2^{1/2})$. This is a characteristic dimension at which the energy of elastic deformation is of the order of the potential barrier of the substrate. This localization indicates that at a distance $R > b_0$ the dislocation stress field localizes in a soliton with a dislocation end. It may be regarded in an incommensurable phase as a superfluous line of the soliton lattice, which breaks off in the new dislocation center in the soliton lattice. A soliton with a dislocation end (shaded area) is shown in Fig. 1. (The lines represent the planes of atoms.) Similar solutions (solitons based on defects) were obtained for superfluid ^{3}He phases by Mineyev and Volovik.[6] The temperature of the phase transition is determined by the characteristic interaction energy of the dislocation pairs. This energy is uniquely related to the elastic constants of the Hamiltonian (2), which is isomorphic relative to the Hamiltonian of the XY model. The

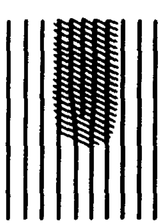

FIG. 1. A soliton with a dislocation end.

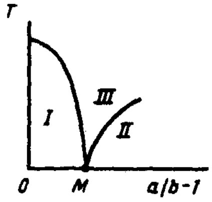

FIG. 2. Phase diagram.

transition temperature can be easily determined from the known results for the XY model.[5] Its dependence on the concentration of adatoms in metallic substrates has the form

$$T_c \sim (v\lambda_2)^{1/2}(1-c)^{-1}b^2\exp\left(-\frac{1}{2}v^{1/2}\lambda_1^{-1/2}(1-c)^{-1}\right).$$

The translational order vanishes as a result of the transition under consideration. The orientational order (direction of solitons), which is defined by the anisotropy of the adfilm, remains after the transition. Therefore, the soliton lattice melts into a soliton liquid crystal. The fact that a two-dimensional crystal melts into a liquid crystal was demonstrated by Nelson and Halperin.[7] The phase diagram for a free lattice is shown in Fig. 2. Phase I represents a commensurable crystal, phase II represents an incommensurable crystal, and phase III is a soliton liquid crystal. The phase diagram in Fig. 1 has a singular point M, which is called a multicritical point. The existence domain of a commensurable phase in a compressed lattice can be compressed into a line ($a = b$).

To verify the obtained phase diagram experimentally, we must investigate the dependence of the magnitude and location of the superstructure reflections of a soliton lattice on the concentration and temperature. In addition to verification of the relation (3), such experiments will make it possible to investigate the mechanism of two-dimensional melting directly.

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