Substrate defects and commensurate-incommensurate phase transition in adsorbed films

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The soliton density index is calculated near the point of the transition from a commensurate phase to an incommensurate phase in adsorbed films in the presence of a random arrangement of point defects in the substrate. This index is 5/6 and very different from that (1/2) of an ideal substrate.

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At degrees of surface coverge approaching multilayer coverage, atoms adsorbed on a crystal surface form lattices with lattice constant which are incommensurate with those of the substrate.[1] Near the point of the transition from the commensurate to the incommensurate phase, the latter consists of large regions of commensurate phase separated by linear regions of a disrupted commensurability—domain walls or solitons—which compensate for the difference between the lattice constants of the film and the substrate[2] (Fig. 1). A typical experimental situation is an adsorbate at equilibrium with a gas in a chamber.[3] If a soliton is to form, the chemical potential of the gas, μ, must exceed a certain critical μ_c.

As μ is increased further (by increasing the pressure, for example[3]), a finite density of solitons n appears in the system. This density can be determined by measuring the shift of the diffraction features of the lattice of adsorbed atoms. Pokrovsky and Talapov[4] have shown that fluctuational displacements of solitons may cause $n(\mu)$ to be a power function $n \propto (\mu - \mu_c)^{s'}$, where s' (the soliton density index) is 1/2. This result has been confirmed experimentally.[3,5]

There is always a finite concentration of point defects on a substrate. These defects may be impurity atoms, vacancies, etc. Their mobility may be extremely low at experimental temperatures[6]; i.e., they may be "frozen." Experiment shows that the defect concentration c will be $c \gtrsim 10^{-3}$ even after a thorough cleaning.[6] At small values of n, the defects may therefore be important. A soliton is a density wave of a finite width Δ_0 (Fig. 1), so that a point defect of the substrate will interact with a soliton in a region of dimension $\propto \Delta_0$. The particular shape of the defect potential is determined by the interaction of the adsorbed atoms with the defect and by the shape of the soliton. For the results of the present letter, however, where we are considering the soliton fluctuations at large distances, the only important point is that the potential of the defect must be a local potential, confined to a region with a width of order Δ_0. The shape of the potential does not appear in the calculations, and in the analysis of the influence of thermal fluctuations the particular potential (Gaussian) is chosen for convenience in the calculations.

Let us consider the effect of defects in the very simple case of a banded soliton

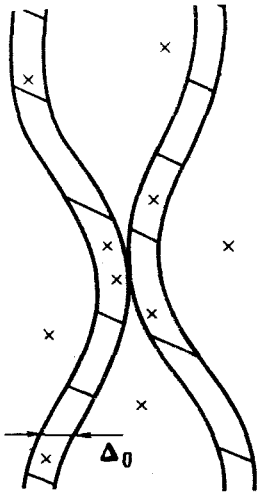

FIG. 1. Banded structure of solitons in the field of point defects (crosses). The hatching shows the region of the solitons.

structure (Fig. 1). A structure of this sort should arise, for example, in the incommensurate lattices which are formed by compressing commensurate lattices along one of the substrate directions.[7] A banded structure has been observed experimentally in the system of freon and exfoliated graphite.[8] The displacement of an isolated soliton in the absence of defects can be described by the Hamiltonian

$$H_0 = \frac{1}{2} \int \lambda (\partial\phi/\partial x)^2 dx . \tag{1}$$

Here λ is the elastic energy per unit length of the soliton. If $T \neq 0$, the mean square displacement of the soliton is $\langle(\phi(x) - \phi(0))^2\rangle = 2T|x|/\Delta$. In the presence of "frozen" defects, a soliton will undergo displacements in a fluctuational manner even at $T = 0$, because of inhomogeneities in the defect distribution. The number (N) of defects which interact with a soliton over a distance L is $N \sim c\Delta_0 L$, and the average magnitude of the fluctuations in the number of defects is $\sim\sqrt{N}$. If the amplitude of the defect potential is v_0, then the energy of the pinning of the soliton by impurities is $W(L) \sim v_0\sqrt{N} \sim v_0\sqrt{c\Delta_0 L}$. Equating this energy to the elastic strain energy (E) of the soliton over the distance L, $E \sim \lambda(\phi/L)^2 L$, we find the estimate $\langle(\phi(L) - \phi(0))^2\rangle \sim v_0\lambda^{-1}(\Delta_0 c)^{1/2} L^{3/2}$. The fluctuations in the displacement caused by the defects thus increase more rapidly than the thermal fluctuations with increasing L. The thermal fluctuations should attenuate the effect of the defects, since they "push" a soliton out of the most favorable configuration. An analysis at $T \neq 0$ can be carried out conveniently in a model with a Gaussian defect potential (the assumption of this particular potential does not restrict the applicability of the results). For this purpose we consider a perturbation V of a Hamiltonian H_0 of the following type (we take the lattice constants of the adsorbed atoms to be 1):

$$V = \int dx \sum_{\phi_0(x)} v_0 \exp\left(-\frac{(\phi(x) - \phi_0(x))^2}{2\Delta_0^2}\right) . \tag{2}$$

Here $\phi_0(x)$ are the coordinates of the randomly positioned defects. We write the free energy as a series in V for an arbitrary defect distribution. After taking the average of the free energy over the coordinates of the frozen defects, the first nonconstant term arises in second order in V; it is

$$<v_0^2\, c\, \Delta_0 T^{-1} \int dx\ \exp\left(-\frac{\phi^2(x)}{4\Delta_0^2}\right)>_{H_0}. \tag{3}$$

Here the angle brackets denote an average over ϕ with the Hamiltonian H_0. The potential (3) is linear in c. The corrections of higher order in c are small if $\Delta_0 c \ll 1$, i.e., if the probability for the appearance of two defects over the width of the soliton is low. The quantity $v_0^2 c\Delta_0 = W_0^2$ represents the mean square pinning energy. It was shown above for the case $T=0$ that this quantity increases linearly with the size of the region. For an analysis of the situation at $T \neq 0$, we perform a transformation analogous to a renormalization in (3). For this purpose we integrate over the short-wavelength Fourier components of the field ϕ with wave vectors in the interval from q_0 to $q' = q_0 \xi^{-1}$ (q_0 is the cutoff momentum), and we then change the scale. This procedure does not alter the functional form of (3), but w_0 and Δ_0 are renormalized. Specifically,

$$W^2(\xi) = W_0^2\, \zeta \frac{\Delta_0}{\Delta};\quad \Delta^2 = \Delta_0^2 + \frac{2T}{\lambda q_0}(\zeta - 1). \tag{4}$$

This result agrees with the rough calculations carried out for $T=0$ if at $T \neq 0$ the asymptotic behavior of W at large values of ξ (i.e., L) is different: $W \propto L^{1/4}$. This means that $\langle(\phi(L) - \phi(0))^2\rangle \sim v_0 \Delta_0 c^{1/2} \lambda^{-3/4} T^{-1} L^{5/4}$ at sufficiently large L; i.e., the displacement fluctuations caused by the defects remain stronger than the thermal fluctuations. If the soliton density n is finite, the displacements of a single soliton are limited to the magnitude $l = 1/n$. This displacement corresponds to the length $L_c \propto l^{8/5}$. The density of the additional energy associated with the finite soliton density is $\lambda (l/L_c)^2 \propto ;^{-6/5}$. As a result, the free energy of the soliton structure can be written

$$F = (\mu_c - \mu)/l + A\left(\frac{v_0^8\, \Delta_0^8\, c^4}{T^2 \lambda}\right)^{1/5} l^{-11/5}, \tag{5}$$

where A is a constant. Minimizing (5) with respect to l, we find the function $n(\mu - \mu_c)$ to be $n \propto (\mu - \mu_c)^{5/6}$. We mentioned above that the index 1/2, corresponding to an ideal substrate, has been observed experimentally. The apparent explanation is that those measurements were taken quite far from the transition point, in a region where the defect contribution to the fluctuations in the soliton displacement was small in comparison with the thermal contribution. The results derived in the present letter mean that when the measurement interval is moved closer to the transition point the index of 1/2 should give way to an index of 5/6.

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