Localization of solitons in adsorbed films

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We analyze how line surface defects of the substrate crystal affect the correlation characteristics of the solitons which form in adatom lattices which are incommensurable with the substrate. Randomly arranged "frozen" defects always localize solitons. The width of the localization region is studied as a function of various parameters. Some experimentally verifiable consequences of localization are pointed out.

1. Incommensurable structures are presently an active field of research. Among the systems of this type are the lattices of atoms which are adsorbed on the surface of a crystal substrate and which have periods incommensurable with those of the substrate. Structures of this type are extermely numerous and are seen in a huge number of adsorbate-substrate systems. Consequently, interest in these systems stems from not only purely physical considerations but also practical considerations. An understanding of the behavior of such systems is necessary for reaching an understanding of many surface processes.

Near the point of commensurability, incommensurable lattices consist of large regions of a phase which is commensurable with the substrate, separated by linear regions in which the commensurability is disrupted—domain walls or solitons. Recent experiments, including some direct diffraction experiments,[1] have revealed several facts which confirm the existence of a soliton superstructure in adsorbed films. A detailed theory has been worked out for soliton superstructures on an ideal (defect-free) substrate (see the reviews in Refs. 2–4). However, we know that defects may play a dominant role in the behavior of few-dimensional systems. At the surface of the crystal there are both point defects (vacancies, impurities, etc.) and line defects (steps). The effect of point defects was studied in Refs. 5–7. In the present paper we examine the effect of a random arrangement of line defects on the behavior of an individual soliton. This is a problem of current interest because defects may play a crucial role in the dynamics of solitons, as experiments have shown.[8] The problem of a soliton in the field of line defects is also of methodological interest, since it may be studied both by renormalization-group transformations and by reduction to the $1D$ quantum-mechanical problem of a particle in a random potential.

In Section 2 we formulate the model of the lattice of adatoms and of substrate defects which we will use. In Section 3 we examine localization in the case of a single potential well. In Section 4 we do the same for the case of randomly positioned potential wells or barriers at high temperatures. In that section we also point out some consequences of soliton localization which would be verifiable experimentally.

2. As a model of the incommensurable lattice of adatoms we choose a system in which the periods of the adsorbed film and those of the substrate are commensurable along the x direction but incommensurable along y; this is a model of an anisotropic crystal.[2–4] In the weak potential relief of the substrate, the energy of the adsorbed film can then be written

$$H=\int dx\,dy\left\{\frac{1}{2}\lambda(\nabla u)^2+w\left[1-\cos\left(\left(\frac{2\pi}{b}-\frac{2\pi}{a}\right)y+\frac{2\pi}{b}u\right)\right]\right\}. \tag{1}$$

Here λ is the elastic constant of the adsorbed film, a is the period of this film, b is the period of the substrate, u is the displacement of an adatom along the y axis, and w is the amplitude of the potential relief of the substrate. A detailed description of the model and many examples of experimental systems which it describes are given in the reviews in Refs. 2–4. A soliton in this model is a density wave of width $l_0 \sim b(\lambda/w)^{1/2}$ along the y axis, which is extended along the x axis. This wave is described in the continuous approximation by

$$u=\frac{2b}{\pi}\operatorname{arctg}\left\{\exp\frac{2\pi y}{b(\lambda/w)^{1/2}}\right\}. \tag{2}$$

Direct substitution easily shows that the energy of the soliton does not depend on its position on the surface. An individual soliton can thus be described by the Hamiltonian

$$H_0=\frac{1}{2}\int dx\,J(\nabla\varphi)^2. \tag{3}$$

Here $\varphi(x)$ is the displacement of the soliton along the y axis at the point x, and $J \sim (\lambda w)^{1/2}a$ is the corresponding elastic constant.

Steps on the surface of the crystal are typical defects, and their effects on adsorption, diffusion, etc., have been studied by many investigators (see the review by Wagner[9]). Steps would not necessarily be natural defects of a crystal surface (growth steps); they can also be produced artificially, and this can be done with a high density on so-called vicinal surfaces.[9] We consider steps which extend along the x axis, i.e., in the same direction as the soliton. This model corresponds completely to the experimental situation on anisotropic crystal faces, where incommensurable crystals of the type under consideration here are observed.[9] If the directions of the steps instead make some angle with the direction of the soliton, the problem essentially reduces to the point-

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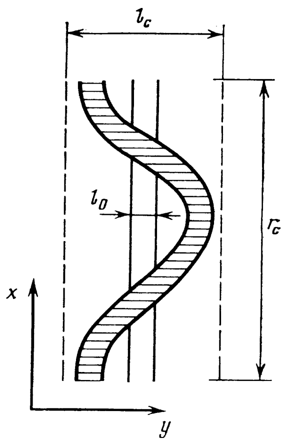

FIG. 1. Pinning of a soliton by an isolated potential well. The well is indicated by the parallel solid lines. The region of the soliton is the hatched region. The dashed lines show the localization band.

defect problem studied in Ref. 6. Fluctuations of the displacement of a step from the x axis are unimportant, as we will show below (Section 3), since the soliton itself fluctuates much more substantially. As a rule, steps are potential wells for adatoms.[9] The simplest model potential of a step is

$$v=v_0[1-\cos(2\pi u/b)]. \tag{4}$$

Substituting the single-soliton solution (2) into this expression, we find an expression for the soliton pinning potential:

$$v=v_0\,\mathrm{ch}^{-2}\left[\frac{2\pi y}{b(\lambda/w)^{1/2}}\right]. \tag{5}$$

We see that a step is a well (or barrier) of width $\sim l_0$ for a soliton and extends along the x axis (Fig. 1). The local nature of the step potential is its most characteristic feature. For convenience in the calculations, we choose a potential of a slightly different form, but one which is still localized in a band of width l_0; specifically, we choose a potential of Gaussian shape. The contribution of the step potential to the Hamiltonian of the soliton-step system is then

$$V=\int dx v_0\exp(-\varphi^2/2l_0^2). \tag{6}$$

The same functional dependence of the defect potential on the coordinate y was used in Refs. 5 and 6.

3. We consider the situation in which there is only a single defect: a potential well extended along the x axis. The Hamiltonian of the problem is then of the form $H = H_0 + V$, where H_0 and V are defined in (3) and (6). For the analysis it is convenient to reduce the problem to a $1D$ quantum-mechanical problem. The rules by which this transformation of the problem is made are as follows.[10,11] The Hamiltonian H is associated with the quantum-mechanical Hamiltonian

$$\tilde{H}=-\frac{T^2}{2J}\frac{d^2}{d\varphi^2}+v(\varphi). \tag{7}$$

The field correlation function φ is expressed in terms of matrix elements,

$$G(x)\equiv\langle\varphi(x)\varphi(0)\rangle=\sum_n\exp\left(-\frac{E_n-E_0}{T}x\right)|\langle 0|\varphi|n\rangle|^2, \tag{8}$$

where E_n are the energy levels of Hamiltonian (7). Clearly, a soliton will be at the bottom of the well at $T = 0$. As the temperature increases (correspondingly, as the quantum fluctuations grow), the amplitude of the soliton fluctuations grows, and the energy of the ground state vanishes, $E_0 \to 0$. In a one-dimensional well, however, there is always a level with an energy[12]

$$E_0=-\frac{J}{2T^2}\left[\int v(\varphi)\,d\varphi\right]^2<0. \tag{9}$$

If $v(\varphi)$ corresponds to (6), we have the following expression for E_0:

$$E_0=-\pi(J/T^2)v_0^2l_0^2. \tag{10}$$

The presence of a level in the well means that outside the well the wave function decays exponentially; i.e., the soliton is localized near the well at any temperature. The width (l_c) of the localization region (Fig. 1) is determined by the argument of the exponential function in the wave function of the bound state. In the high-temperature limit we have

$$l_c=(2/\pi)^{1/2}T^2/Jv_0l_0. \tag{11}$$

The correlation function $G(x)$ behaves in accordance with $\exp(-|x|/r_c)$, where r_c (Fig. 1) is the distance over which a soliton is trapped by the well potential:

$$r_c=T^3/\pi Jv_0^2l_0^2. \tag{12}$$

We will now show how the same results can be derived by a renormalization-group approach. We return to the Hamiltonian $H = H_0 + V$ in (3) and (6). The free energy F is

$$F=-T\ln\int\prod_x\mathscr{D}\varphi(x)\exp\left(-\frac{H_0+V}{T}\right). \tag{13}$$

Expanding (13) in powers of V/T, we find the average energy of the pinning by a well:

$$\left\langle\int dxv(\varphi)\right\rangle_{H_0}=\left[\int\prod_x\mathscr{D}\varphi(x)\exp\left(-\frac{H_0}{T}\right)\int dxv(\varphi)\right]\times\left[\int\prod_x\mathscr{D}\varphi(x)\exp\left(-\frac{H_0}{T}\right)\right]^{-1}. \tag{14}$$

We make a transformation analogous to the renormalization-group transformation[13] in (14). In φ we pick out a quantity φ_1, as follows:

$$\varphi=\varphi_0+\varphi_1,\quad \varphi_1=\int_{q_0}^{q_1}dq\varphi_qe^{iqx},\quad q_0=\frac{2\pi}{a}. \tag{15}$$

We integrate over φ_1 in (14) and change the scale:

$$x'=\zeta x,\quad \zeta=q_0/q_1. \tag{16}$$

Since the potential is of Gaussian shape, its shape is not changed by this transformation; there is simply a renormalization of v_0 and l_0:

$$v_0\to v_0\zeta\frac{l_0}{l},\quad l_0\to l,\quad l^2=l_0^2+\frac{2Ta}{\pi J}(\zeta-1). \tag{17}$$

The physical meaning of (17) is simple: The probability for finding a soliton in a well is $\sim l_0/l$, and the corresponding binding energy for the binding of a "piece" of the soliton of length ζa with the well is of order $\zeta a v_0 l_0/l$, where l is determined by the expression for a freely fluctuating soliton. It can be seen from (17) that the integration over the short-wave components leads to an increase in pinning potential (6). The energy (E) of the fluctuations of the free soliton described by Hamiltonian (3) decreases in accordance with

$$E \sim J(\varphi/\zeta a)^2 \zeta a \sim J(\varphi^2/\zeta a).$$

At a certain $\zeta = \zeta_c$ the energies E and V become comparable. Equating them, we find expressions for ζ_c, i.e., for $r_c = \zeta_c a$ and l_c:

$$l_c^2 \sim 2Tr_c/\pi J, \quad r_c \sim T^3/Jv_0^2 l_0^2. \tag{18}$$

We thus find values of l_c and r_c which agree with the exact values in (11) and (12). This example shows that the renormalization-group approach makes it possible to derive the correct results in the high-temperature limit through an analysis of a perturbation-theory series.

How do fluctuations of the displacement of the well affect the results derived above? Here it is convenient to take the renormalization-group approach. The step is a one-dimensional entity, and its fluctuations can be described by a Hamiltonian of the type in (3). Its stiffness J_s, however, must be significantly greater than J, because the interaction energy between substrate atoms is at least an order of magnitude greater than the adatom interaction energy (the difference would be by several orders of magnitude in the case of an inert-gas adsorbate). The fluctuations of the displacement of the step are thus determined by the same law as that which determines the displacements of the soliton, (17), but these fluctuations are considerably smaller in amplitude. Since the displacement of a step results from a diffusion of substrate atoms, this process is exceedingly slow at temperatures not too close to the melting point of the substrate. We may thus treat the steps as frozen defects with respect to a soliton. Formally, we can introduce a dependence on the well coordinate, $\varphi_0(x)$, in the potential (6), using the substitution

$$\int dx v(\varphi(x)) \to \int dx v(\varphi(x) - \varphi_0(x)).$$

We take the average of free energy (13) (the defects are frozen) over φ_0 with a Hamiltonian of the type in (3). As a result we find an increment in the expression for l^2 in (17), a term $Ta(\zeta - 1)/\pi J_s$, which is small in comparison with the contribution from the soliton fluctuations. We will therefore assume everywhere below that the steps do not fluctuate.

4. It was shown above that a soliton is always localized at an isolated potential well. If the wells are arranged in a strictly periodic fashion, however, the soliton becomes delocalized. This result can be understood easily by considering the quantum-mechanical analogy. A level of an isolated well is "smeared out" into a band in a periodic potential relief, and the wave functions become delocalized. If, on the other hand, the strict periodicity in the arrangement of wells is disrupted, we know that a localization will occur (Ref. 14, for example). A soliton will therefore be localized even if there is a finite density of randomly positioned steps.

The expressions for the width of the localization band will of course depend on the particular potential, the temperature, and so forth. In this section of the paper we consider the high-temperature case, in which the width of the localization band is significantly greater than the average distance between steps. Since the effect arises in second order in v_0, the results do not depend on the sign of v_0. In this case the energy of the interaction with the substrate is

$$V = \int dx \left\{ \sum_{\varphi_0} v_0 \exp\left[-\frac{1}{2l_0^2} (\varphi(x) - \varphi_0)^2 \right] \right\}. \tag{19}$$

Here φ_0 represents the coordinates of the steps. We take the renormalization-group approach. The first nonconstant correction to the free energy arises in second order in v_0, and is given by the following expression, before we take an average over the step coordinates φ_0:

$$\Delta F(\varphi_0) = \left\langle \frac{v_0^2}{2T} \int dx\, dx' \exp\left\{ -\frac{1}{2l_0^2} [(\varphi(x) - \varphi_0)^2 + (\psi(x') - \varphi_0)^2] \right\} \right\rangle_{\varphi,\psi}. \tag{20}$$

Here the angle brackets denote an average over the fields φ and ψ with Hamiltonian H_0 in (3). If (Section 3) the condition $l_c \gg l_s$ holds, where l_s is the average distance between steps, the averaging over the positions of the steps reduces to an integration over φ_0. As a result we find

$$\Delta F = \left\langle \frac{\pi^{1/2} v_0^2}{2T} \frac{l_0}{l_s} \int dx\, dx' \exp\left\{ -\frac{1}{4l_0^2} [\varphi(x) - \psi(x')]^2 \right\} \right\rangle_{\varphi,\psi}. \tag{21}$$

In deriving (21) we have implicitly assumed $l_s \gg l_0$, which is obviously irrelevant to the conclusion that localization occurs. We now use the fields φ and ψ simultaneously to carry out the transformation described in Section 3. As a result we find

$$v_0^2 \to v_0^2 \zeta^2 l_0/l, \quad l^2 = l_0^2 + 2Ta(\zeta - 1)/J. \tag{22}$$

Repeating the arguments in Section 3, we find expressions for the width of the localization band, l_c, and the trapping distance r_c:

$$l_c^3 \sim T^4 l_s/J^2 v_0^2 l_0^2, \quad r_c = Jl_c/2T. \tag{23}$$

As in the preceding section, these results can be defended on the basis of $1D$ quantum mechanics. For this purpose we use an expression for the localization distance of a particle in a "white noise" potential. This question is analyzed in detail in the book by Lifshits *et al.*[14] In the units used in Ref. 14, the Schrödinger equation is

$$-\frac{d^2\Psi}{d\varphi^2} + U(\varphi)\Psi = E\Psi, \tag{24}$$

$$U(\varphi) = \frac{2J}{T^2} \sum_{\varphi_0} v(\varphi - \varphi_0). \tag{25}$$

If the localization length (corresponding to l_c in our case) satisfies $l_c \gg l_s$, potential (25) may be regarded as a white noise. It is customary to characterize such a potential by the quantity[14]

$$D = \frac{1}{2} \int d\varphi \langle U(\varphi) U(0) \rangle_{\varphi_0}, \tag{26}$$

which can easily be calculated. As a result we find, for potential (6),

$$D=4\pi J^2 v_0^2 l_0^2 / T^4 l_s. \tag{27}$$

The localization length is[14] $l_c = 4E_c/D$, where E_c is the energy of a particle. In these units, the energy of a particle localized in a region of size l_c is $E_c \sim l_c^{-2}$. We thus find an expression for l_c which is the same as (23).

In summary, it follows from these calculations that solitons localize at line defects, even at high temperatures. This circumstance has some experimentally verifiable consequences. One concerns the soliton density index. At a commensurable-incommensurable phase transition, the soliton density n varies with the chemical potential of the gas in the chamber, μ, in accordance with either $n \propto (\mu - \mu_c)^s$ or $n \propto \ln^{-1}(\mu - \mu_c)$ with $s = 0$ (Refs. 2–4). Here μ_c is that value of the chemical potential at which solitons first form. The soliton density index s is determined by the extent to which the soliton interaction energy falls off over distance. For a clean substrate at $T = 0$ we would have $s = 0$ (Refs. 15 and 2–4), since in this case the solitons interact exponentially weakly. If the substrate is ideal, and $T \neq 0$, the interaction between solitons is of a power-law nature because of thermal fluctuations, and we have $s = 1/2$ (Refs. 16 and 2–4). For a substrate with point defects at $T \neq 0$ we have $s = 5/6$, since in this case the fluctuations caused by the nonuniform arrangement of defects dominate.[6] In the case of a substrate with a significant density of line defects, e.g., a vicinal surface,[9] localized solitons will interact exponentially weakly even at high temperatures. This circumstance may give rise to a behavior $n \propto \ln^{-1}(\mu - \mu_c)$, by analogy with the case of the exponentially weak interaction at $T = 0$ on a clean substrate.[15]

The localization of a soliton means that an infinite soliton cannot move over the substrate even in an arbitrarily weak random potential. In this case, displacements of a soliton can occur only as a result of its rupture, followed by a motion of the resulting "pieces." We will not go into this process in detail here; we simply note that in the limit $T \rightarrow 0$ the activation energy for the displacement of a soliton, even in a weak potential relief, is determined by the soliton rupture energy, as in the case of strong pinning by defects.[17]

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