Loss-Free Dislocation Motion in a Lattice Model*

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It is shown that a mode of dislocation motion exists in the modified Frenkel-Kontorova model in which the dislocation moves at a high constant speed without exciting any lattice waves and with no applied stress required to maintain the motion. The Peierls stress, σ_P, for the model parameters employed has the value $\sigma_P = 0.0506\mu$, with μ the shear modulus, so that this result provides an example of a dislocation subject to a periodic Peierls potential in its steady motion, without this fact giving rise to radiation losses.

The important role of dislocations in the plastic flow of crystalline solids is due to the high mobility of these crystal defects. There are, however, various loss mechanisms which produce an effective drag on a moving dislocation and an applied stress field must supply energy to it in order to maintain its motion.

Even if one excludes consideration of all other loss mechanisms, such as those caused by dislocation interaction with electrons, phonons, other defects, etc., there remains the energy that is carried away by the lattice waves generated directly by the moving dislocation itself. Various calculations[1-4] on different lattice models have exhibited this mode of energy loss and it has come to be regarded as an inherent characteristic of dislocation motion.

Here we report on a mode of dislocation motion in the modified Frenkel-Kontorova model in which the dislocation moves at a high constant speed without exciting any lattice waves and with no applied stress required to maintain the motion.

The model employed in these calculations is shown in Fig. 1. It differs from that originally introduced by Frenkel and Kontorova[5] by replacement of the sinusoidal substrate potential by one that is piecewise quadratic and it has been used in several previous studies of stationary[6,7] and moving dislocations.[1,2] For a dislocation moving under an applied stress σ in steady-state conditions with velocity v, the displacement $x(t)$ of a typical atom from the well bottom from which it began before the passage of the dislocation satisfies the equation[8]

$$d^2x/dt^2 = x(t+v^{-1}) - 2x(t) + x(t-v^{-1}) + F(x(t)) + \sigma, \tag{1}$$

where $F(x)$ is the piecewise linear force on the atom due to the substrate potential and is defined for the range of x of interest here by the equations

$$F(x) = \begin{cases} -Px, & -\gamma \le x \le \gamma, \\ -Q(\frac{1}{2} - x), & \gamma \le x \le 1-\gamma, \\ P(1-x), & 1-\gamma \le x \le 1+\gamma. \end{cases} \tag{2}$$

Here we are employing units in which the lattice parameter, the atomic mass, and the longitudinal spring constant are all unity. P is the ratio of the substrate spring constant to the longitudinal spring constant (corresponding in the model crystal to the ratio of shear to tensile modulus), γ (Fig. 1) corresponds to the critical shear stress of the perfect crystal, and $Q = 2\gamma P/(1-2\gamma)$. In the units employed, $v_s = 1$, where v_s is the macroscopic (i.e., long-wavelength-limit) sound velocity for the model.

We now seek a nontrivial solution to Eq. (1) with the applied stress $\sigma = 0$ and, guided by computer-

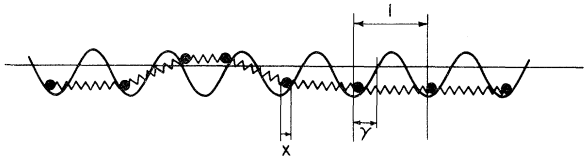

FIG. 1. Modified Frenkel-Kontorova model. Horizontal line separates the portions of the piecewise quadratic potential with positive and negative curvatures; γ is the distance from the potential well minimum to the point of change of curvature.

simulation studies, we make the *a priori* assumption that it satisfies the relation $x(t) = 1 - x(-t)$, where the origin of the time scale is chosen so that $x(0) = \frac{1}{2}$. As in our previous work on this model,[8] it is convenient to employ the two-sided Laplace transform defined by

$$X(s) = \int_{-\infty}^{\infty} e^{-st} x(t)\, dt, \tag{3}$$

and it may be shown[9] that

$$X(s) = \frac{Pe^{-s\alpha} - Q\sinh(s\alpha) + s(P+Q)\int_{-\alpha}^{\alpha} x(t)e^{-st}\, dt}{sD(s)}, \tag{4}$$

where

$$D(s) = s^2 + (2+P) - 2\cosh(sv^{-1}), \tag{5}$$

and $\alpha > 0$ is defined by the relation

$$x(\alpha) = 1 - \gamma. \tag{6}$$

By consideration of the inverse transform of Eq. (4) it is found that a formal solution to the problem may be written, for $t > 0$, as

$$x(t) = 1 - \sum_{i=1}^{\infty} [c_i \exp(s_i t) + c_i^* \exp(s_i^* t)], \tag{7}$$

where the complex numbers s_i are the zeros of $D(s)$ which lie in the second quadrant of the complex plane, excluding those that are purely imaginary, and the complex numbers c_i must satisfy the infinite set of linear equations

$$c_i = \frac{(P+Q) - Q\cosh(s_i\alpha) + s_i(P+Q)\sum_{j=1}^{\infty}[c_j f(s_i, s_j, \alpha) + c_j^* f(s_i, s_j^*, \alpha)]}{2s_i[s_i - v^{-1}\sinh(s_i v^{-1})]}, \quad i = 1, 2, \ldots, \tag{8}$$

where

$$f(s_i, s_j, \alpha) = (s_i^2 - s_j^2)^{-1}\{\exp(s_j\alpha)[(s_i - s_j)\exp(s_i\alpha) + (s_i + s_j)\exp(-s_i\alpha)] - 2s_i\}.$$

Finally, the *a priori* symmetry condition put on the solution and the requirement that there are no traveling lattice waves generated both demand that

$$\sum_j \operatorname{res}(X(s)e^{st}) = 0, \tag{9}$$

where the summation is carried out over all the purely imaginary zeros of $D(s)$.

Equations (6), (8), and (9) form an infinite set for the determination of the quantities v, α, c_1, $c_2, \ldots$. We have not examined the question of convergence theoretically, but have considered the approximate solutions v_N, α_N, $c_{1,N}, \ldots, c_{N,N}$ obtained by truncating the infinite series in Eqs. (7) and (8) at $i, j = N$ and then considering only the finite set $i = 1, \ldots, N$ of Eqs. (8). We have carried out this process explicitly for the case $P = 0.25$ and $\gamma = 0.35$ with the results $v_1 = 0.2574$, $v_2 = 0.2512$, and $v_3 = 0.2509$ and with correspondingly close agreement between the functions $x_1(t)$, $x_1(t)$, and $x_3(t)$. They are shown in Fig. 2 and, on this scale, are indistinguishable. The monotonic character of the zero-stress solution and the absence of generated lattice waves should be noted.

In order to study the stability of this solution, a computer simulation of the model was made, using the numerical techniques previously described,[8] with initial atom displacements and velocities corresponding to the function $x_3(t)$. With zero applied stress, the computer simulation showed that the dislocation continued to move with a measured velocity $v = 0.251 \pm 0.001$ for the

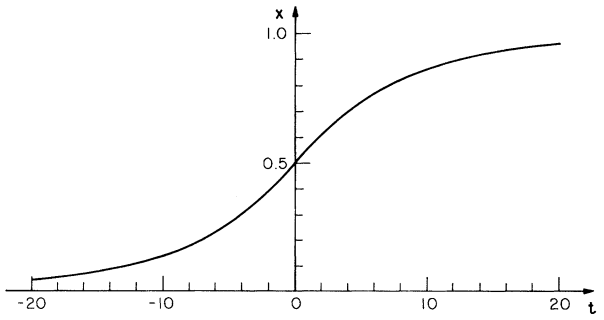

FIG. 2. Atomic displacement function $x(t)$ for steady, loss-free motion.

length of the test in which the dislocation traversed a distance of 40 lattice parameters. The computer simulation determination of $x(t)$ cannot be distinguished, on that scale, from that shown in Fig. 2. In another computer simulation of the model, the dislocation was first brought to steady conditions under an applied stress with $v = 0.660$, and the stress then gradually reduced. At the time the stress reached zero, the measured dislocation velocity was $v = 0.275$. After that time, it decreased very slowly so that after traversal of 65 lattice parameters under zero stress, at which time the computer simulation was terminated, the dislocation velocity had declined only to $v = 0.264$. The velocity trend appeared to be approaching $v = 0.25$ asymptotically. We conclude, therefore, that the loss-free mode can be attained in a natural manner.

It should be noted that the Peierls stress, σ_P, for this model, and the values of the model parameters here assumed, does not vanish. Rather, for $P = 0.25$ and $\gamma = 0.35$, the general theory[6,7] gives $\sigma_P = 0.0506\mu$, where μ is the shear modulus of the crystal. Therefore, contrary to the frequent assumption,[10] the fact that the dislocation is subject to a periodic Peierls potential in its steady motion does not inevitably give rise to radiation losses, at least for the modified Frenkel-Kontorova model studied here. Whether such loss-free motion is possible in other models is a subject for further investigation, but in any case the present work demonstrates that the relationship between radiation losses and the periodic Peierls potential is not straightforward. The dynamic Peierls stress,[1] σ_{PD}, for these parameters also has a nonzero value, namely $\sigma_{PD} = 0.7520 \times 10^{-3}\mu$. Therefore the result previously stated,[1] based on the local-mode approximation, that steady dislocation motion is possible only for $\sigma > \sigma_{PD}$ is incorrect for the case when one starts with steady motion at $\sigma > \sigma_{PD}$ and then slowly reduces the stress level. On the other hand, for the case of a dislocation starting from rest in an unstable configuration under an applied stress σ, it is necessary for $\sigma \gtrsim \sigma_{PD}$ for continued motion to occur.[9]

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Diamagnetic Susceptibility of Tetrahedral Semiconductors*

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The lattice contribution to the diamagnetic susceptibility, χ_L, is written as a sum of three terms, a core term χ_c, a Langevin-like valence-electron contribution χ_v, and a Van Vleck paramagnetic term χ_p using a one-oxcillator model. Measurements of χ_L and $d\chi_L/dT$ for diamond, Si, Ge, GaAs, and GaP are presented. The model allows a separate determination of each of the three terms and relates these terms to the symmetry and extent of the valence-bond charge distribution.

The purpose of this Letter is to show that chemical bonding and the diamagnetism of semiconductors are related in a simple way. A model is presented which describes the diamagnetism in terms of three contributions: two Langevin-like diamagnetic terms χ_c and χ_v which arise from the core and va-