tions that the most favorable conditions for the observation of the multimode features are (a) Jahn-Teller coupling of intermediate strength and (b) choice of hosts and impurities such that the vibronic interaction shall scan a wide frequency range in the normal modes. This is best achieved by employing impurity atoms and cations and anions of the host crystal whose masses are all similar and for which the force constants suffer little change by the introduction of the impurity. (Fe^{2+} in cubic ZnSe exemplifies the criteria.)

[1]F. S. Ham, Phys. Rev. 166, 307 (1968). See also F. S. Ham, in *Electron Paramagnetic Resonance*, edited by S. Geschwind (Plenum, New York, 1971).
[2]R. Englman, *The Jahn-Teller Effect in Molecules and Crystals* (Wiley, New York, 1972).
[3]J. C. Slonczewski, Solid State Commun. 7, 519 (1969).
[4]A proof of Eq. (1) has been given by M. C. M. O'Brien, J. Phys. C: Proc. Phys. Soc., London 5, 2045 (1972), for coupling to many vibrational modes, which, however, rests on an unwarranted assumption ($f_0=f_0*$) to be discussed in this Letter. Equation (1) and the range of variation $1>q>0.5$ have also been derived by J. R. Fletcher, J. Phys. C: Proc. Phys. Soc., London 5, 852 (1972), in his approximate treatment of the many-mode coupling.
[5]K. Ždánský, Phys. Rev. 177, 490 (1969).
[6]W. Moffitt and W. Thorson, Phys. Rev. 108, 1251 (1957).
[7]O'Brien, Ref. 4.
[8]Fletcher, Ref. 4.
[9]R. Englman and B. Halperin, J. Phys. C: Proc. Phys. Soc., London 6, L219 (1973).

Can Dislocations be Accelerated through the Sonic Barrier?*

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It has been conjectured, on the basis of the Atkinson-Cabrera solution for the steady motion of a dislocation in a modified Frenkel-Kontorova model, that dislocations can be accelerated from subsonic to supersonic velocities. Computer-simulation results are presented to show that the regular dislocation motion assumed in the Atkinson-Cabrera solution breaks down, and the solution ceases to be valid before the sound velocity is reached.

The question of whether crystal dislocations can be continuously accelerated from subsonic to supersonic speeds is at present open.[1] In this connection, the work of Atkinson and Cabrera[2] is relevant. They have presented an analytical solution for the steady motion of a dislocation in a Frenkel-Kontorova model with piecewise harmonic substrate potential and find a stress dependence of the steady-state dislocation velocity which varies smoothly as its value approaches and exceeds the speed of sound in the linear chain. The Atkinson-Cabrera approach has subsequently been applied to the analysis of the uniform motion of a screw dislocation in a lattice by Ishioka[3] and by Celli and Flytzanis[4] with similar results. Although these calculations are specifically for steady dislocation motion, the absence of singular behavior at the sound velocity does suggest to Ishioka[3] that dislocations in this type of model can be accelerated to supersonic motion. It is the purpose of this Letter to present the results of some computer simulations of the Atkinson-Cabrera model which were made to test this hypothesis.

The linear chain model originally introduced by Frenkel and Kontorova[5] consisted of an infinite line of atoms with harmonic nearest-neighbor interactions with an additional force exerted on each atom by a sinusoidal substrate potential. This substrate potential may be regarded as representing the effect of the remaining atoms of a crystal upon those in the slip plane. For the purpose of greater analytical simplicity, a modified Frenkel-Kontorova model has been employed by Kratochvil and Indenbom[6] and by Weiner and Sanders.[7] In this model the sinusoidal substrate potential has been replaced by a periodic function $U(\bar{\xi})$, with period equal to the lattice parameter b, which is piecewise quadratic of the form

$$U(\bar{\xi})=\tfrac{1}{2}k_2\bar{\xi}^2, \quad |\bar{\xi}|\leq\varphi, \tag{1}$$

$$U(\bar{\xi})=\tfrac{1}{4}k_2\varphi b-\frac{k_2\varphi}{b-2\varphi}\left(\frac{b}{2}-\bar{\xi}\right)^2, \quad \varphi\leq|\bar{\xi}|\leq\frac{b}{2},$$

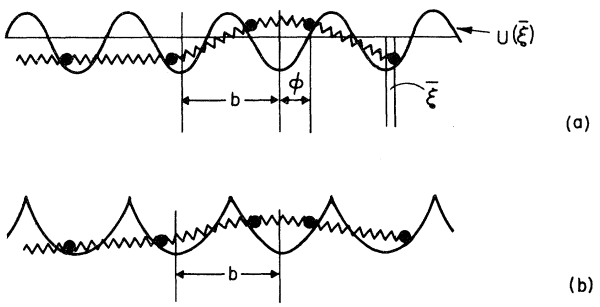

FIG. 1. (a) Modified Frenkel-Kontorova model. A horizontal line separates portions of piecewise quadratic potential with positive and negative curvatures; φ is distance from potential-well minimum to point of change of curvature. (b) Atkinson-Cabrera model corresponding to case $\varphi = b/2$.

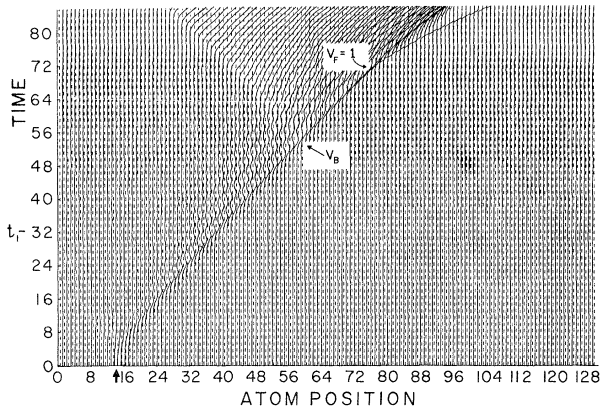

FIG. 2. Computer-plotted atom trajectories for accelerating dislocation. Vertical dashed lines mark boundaries of potential wells [Fig. 1(b)]. Arrow shows initial position of dislocation (two atoms in single well). Stress, initially equal to σ_p, increases linearly with time starting at $t = t_1$. Breakdown of regular dislocation motion occurs when dislocation reaches $v_B = 0.94$ with resulting backward propagation of breakdown wave. Atom collisions begin when front velocity $v_F \simeq 1$ with resulting forward propagation of collision wave.

where $\bar{\xi}$ is the position of a given atom relative to the nearest potential minimum, Fig. 1(a). The substrate potential emplyed by Atkinson and Cabrera corresponds to the choice $\varphi = b/2$, Fig. 1(b). The equation of motion of the model then takes the form

$$m d^2\bar{x}_j/d\bar{t}^2 = k_1(\bar{x}_{j+1} - 2\bar{x}_j + \bar{x}_{j-1}) - k_2\bar{\xi}_j + \bar{\sigma}. \quad (2)$$

Here m is the atomic mass, $\bar{x}_j$ is the position of the jth atom measured from a fixed origin common to all of the atoms, $\bar{\xi}_j$ is the position of the jth atom relative to its nearest potential-well minimum, k_1 is the linear spring constant of the chain, k_2 is the substrate constant as in Eq. (1), and $\bar{\sigma}$ is a force applied to each atom representing an applied shear stress. It is convenient to introduce dimensionless quantities as follows: $x_j = \bar{x}_j/b$, $\xi_j = \bar{\xi}_j/b$, $P = k_2/k_1$, $\sigma = \bar{\sigma}/k_2 b$, and $t = (k_1/m)^{1/2}\bar{t}$. The equation of motion then takes the simpler form

$$d^2x_j/dt^2 = x_{j+1} - 2x_j + x_{j-1} - P\xi_j + P\sigma. \quad (3)$$

In terms of these dimensionless variables $v_\infty = 1$, where v_∞ is the speed of wave propagation for infinite wavelength in the linear chain with the substrate potential neglected.

The computer simulation conditions were as follows: A chain of 131 atoms was employed with the initial dislocation position in the fourteenth well. The value of $P = 0.25$ was chosen to correspond to that employed by Atkinson and Cabrera. For this case the Peierls stress $\sigma_p = \frac{1}{2}[P/(P+4)]^{1/2} = 0.121$. The atoms were initially at rest at positions corresponding to a stress $\sigma = \sigma_p - 1\times10^{-7}$. The imposed stress program for $t > 0$ was $\sigma(t) = \sigma_p + 1\times10^{-7}$ for $0 < t < t_1 = 32.7$, $\sigma(t) = \sigma_p + \alpha(t - t_1)$ for $t > t_1$; $\alpha = 3.81\times10^{-3}$. The period $t_1 = 32.7$ of constant stress was chosen to permit the dislocation velocity to reach its steady-state value. Details of the numerical procedure will be presented elsewhere.[8] At high stress levels the crossing of particle trajectories was found to occur. This physically unrealistic phenomenon is permitted mathematically by the linear springs of the atom chain, and the model was therefore modified to incorporate elastic collisions of atoms when their positions coincided. The computer-plotted (Calcomp system) atom trajectories incorporating this modification are shown in Fig. 2. The following features of the computer results may be noted:

(1) After $t = t_1$ and until breakdown, the dislocation velocity as found by computer is, for a given $\sigma(t)$, within $\pm 1.5\%$ of the Atkinson-Cabrera solution; in other words, the stress variation is sufficiently slow to lead to quasi-steady-state conditions.

(2) When the dislocation velocity reaches the value 0.94, the dislocation breaks down, i.e., the regular dislocation motion exhibited up to that time and postulated in the analytical solution no longer takes place. We refer to the velocity at which this phenomenon takes place as the breakdown velocity, v_B. A similar breakdown phenomenon as the sound speed was approached

was found earlier by Weiner[9] in the computer simulation of the modified Frenkel-Kontorova model with φ [Fig. 1(a)] = $0.3b$. Although it is no longer possible to speak of dislocation velocity past v_B, it is still possible to compute the front velocity v_F, the velocity at which potential-well boundaries are crossed by the lead atom of the disturbed region.

(3) As the stress level continues to increase, and $v_F \to 1$, atom collisions begin to occur.

(4) Two types of waves are caused to propagate through the lattice by these phenomena: (a) a backward-moving breakdown wave, and (b) a forward-moving collision wave.

Several cross checks have been made of the computer-simulation results. (i) The atomic displacements corresponding to the Atkinson-Cabrera solution have been determined analytically, and it is found that they do, in fact, lead to multiple-well crossings, contrary to the *a priori* assumption, at a steady-state velocity $v_B(P)$. (ii) As the rate of stress rise is decreased in the computer-simulation studies, the velocity at which breakdown is first observed decreases and approaches the theoretical value of $v_B(P)$ computed under (i) above. (iii) Computer-simulation runs have been made in which the stress is increased to a value slightly larger than that required for breakdown and is then held constant. Breakdown and the subsequent growth of the extended fault region occurs in much the same manner as in the increasing stress program for Fig. 2. Details of these cross checks will be published elsewhere.[8]

In summary, then, we conclude that the Atkinson-Cabrera solution does *not* provide support for the hypothesis that dislocations may be accelerated to supersonic speeds since it ceases to be valid at velocities greater than $v_B < 1$.

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[1]For a discussion of this question and further references, see J. P. Hirth and J. Lothe, *Theory of Dislocations* (McGraw-Hill, New York, 1968), Chap. 7; or F. R. N. Nabarro, *Theory of Crystal Dislocations* (Oxford Univ. Press, Oxford, England, 1967), Chap. 7.

[2]W. Atkinson and N. Cabrera, Phys. Rev. 138, A763 (1965).

[3]S. Ishioka, J. Phys. Soc. Jap. 30, 323 (1971). See also the computer-simulation results for low dislocation velocity in S. Ishioka, J. Phys. Soc. Jap. 34, 462 (1973).

[4]V. Celli and N. Flytzanis, J. Appl. Phys. 41, 4443 (1970).

[5]J. Frenkel and T. Kontorova, Phys. Z. Sowjetunion 13, 1 (1938), and J. Phys. (U.S.S.R.) 1, 137 (1939).

[6]J. Kratochvil and V. L. Indenbom, Czech. J. Phys. 13, 814 (1963).

[7]J. H. Weiner and W. T. Sanders, Phys. Rev. 134, A1007 (1964).

[8]Y. Y. Earmme and J. H. Weiner, to be published.

[9]J. H. Weiner, Phys. Rev. 136, A863 (1964). For recent dynamical calculations based on this model see J. Tasi, to be published.

Identification of Irradiation-Induced Al-Mn Dumbbells in Al Crystals by Backscattering

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By measuring the energy spectra of backscattered 1-MeV He^+ ions from Al-0.09 at.% Mn crystals, it was found that Mn atoms were displaced from lattice sites by irradiation with 0.3–1.0-MeV He^+ ions at 35°K. Annealing results and an analysis of ⟨110⟩ and ⟨111⟩ axial channeling and {100} planar channeling indicated that the Mn atoms were displaced by trapping irradiation-induced interstitial Al atoms, forming Al-Mn atom pairs in the ⟨100⟩ dumbbell configuration.

An analysis of the spectra of backscattered high-energy ions from single crystals can be used to determine the position of foreign atoms in the host lattice.[1-4] This technique, based on the channeling phenomenon, has been widely applied to the location of ion-implanted impurities in semiconductors[3-6] and in metals.[7-9] Under suitable conditions, the positions of impurity atoms can be determined to within 0.1–0.2 Å, for concentrations as low as 10^{-4} atomic fraction.[4] The method has great potential for studying impurity–point-defect interactions. The application of this