Dislocation Velocities in a Linear Chain*

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Dislocation velocities as a function of applied stress are computed for a modified Frenkel-Kontorova model. The analysis is approximate in that only localized normal modes of motion (local modes) are considered and it is found that steady-state velocities are attained because of imperfect transfer of energy between successive local modes. The significant stress parameter for this model is found to be the dynamic Peierls stress σ_{PD} with the property that dislocation motion will be maintained for any stress $\sigma>\sigma_{PD}$, without the aid of thermal motion, upon condition that the dislocation has surmounted one potential barrier while the stress is applied. For the model parameters here considered, $\sigma_{PD}\sim 10^{-2}\sigma_P$, where σ_P is the static Peierls stress. The model calculations show the extreme stress sensitivity of dislocation velocity at low velocities which has been observed experimentally. Finite-difference calculations show that the local-mode approximation gives reasonably good accuracy up to dislocation velocities approximately 0.7 the speed of wave propagation for infinite wave length in the linear chain.

1. INTRODUCTION

IN a previous paper[1] (to be denoted by I), a modified Frenkel-Kontorova dislocation model[2] was used to study the probability that a dislocation under an applied stress less than the Peierls stress σ_P leaves a given equilibrium position due to thermal motion. Using the same model, we consider here the velocity with which the dislocation will continue to move under stress once it has surmounted the first potential barrier.

This work is motivated by the desire to gain insight into the nature of the stress dependence of dislocation velocities, as experimentally observed for the first time by Johnston and Gilman[3] in LiF single crystals. Theoretical models for this phenomenon have been proposed by Gilman[4] and, more recently, by Celli *et al.*[5] These models contain many aspects of real crystal behavior, such as dislocation kinks and dragging points which are, of course, not included in the Frenkel-Kontorova model. On the other hand, the latter does contain the feature, not directly included in the others, of a discrete atomic structure, and may thus shed some light on the origin of the intrinsic plastic resistance of a crystal whose existence Gilman[4] is led to postulate on the basis of the experimental evidence. While the model is too idealized for quantitative comparison, the results do exhibit some of the qualitative features of the experimental observations. In particular, there is a stress level below which dislocation motion cannot be maintained. This stress, here termed the dynamic Peierls stress σ_{PD} is approximately $10^{-2}\sigma_P$, where σ_P is the static Peierls stress for this model as computed in I. The dislocation velocity is found to be a very sensitive function of stress at low velocities, becoming less sensitive to stress when dislocation velocities approximately $0.1V_\infty$ are reached where V_∞ is the speed of wave propagation for infinite wave length in the linear chain with the substrate potential neglected.

The description and analysis of the model is presented in Sec. 2. The treatment is approximate in that only localized normal modes of motion (local modes) are included. Finite-difference calculations which did not make this approximation were performed on a digital computer in order to check the range of validity of this approximation, and these are described in Sec. 3.

2. MODEL DESCRIPTION AND ANALYSIS

The modified Frenkel-Kontorova dislocation model utilized in I is again employed. It consists of a linear chain of mass points with mass m (hereafter referred to as atoms) interconnected by linear springs with spring constant k_1 and equilibrium spacing b. To represent the effect of the remaining atoms of the crystal, the atoms are subjected to a periodic (with period b) substrate potential $U(x)$, which is continuous, piecewise quadratic and defined as follows:

$$U(x)=\tfrac{1}{2}k_2x^2, \quad |x|\leq\phi$$
$$=\tfrac{1}{4}k_2\phi b-[(k_2\phi)/(b-2\phi)](\tfrac{1}{2}b-x)^2,$$
$$\phi\leq|x|\leq\tfrac{1}{2}b, \quad (2.1)$$

where x is the distance from a potential minimum.

A unit dislocation in this model corresponds to a configuration which has an excess of one atom relative to the number of potential wells in a finite length of the model. An applied shear stress is represented by a force $\bar{\sigma}$ applied to each atom (Fig. 1). The following dimen-

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[1] J. H. Weiner and W. T. Sanders, Phys. Rev. **134**, A1007 (1964), hereafter referred to as I.

[2] The same modification of the Frenkel-Kontorova model has been employed for static calculations by R. Hobart, dissertation, University of Illinois, 1961 (unpublished) and by J. Kratochvil and V. L. Indenbom, Czech. J. Phys. **13**, 814 (1963).

[3] W. G. Johnston and J. J. Gilman, J. Appl. Phys. **30**, 129 (1959). Similar results for other materials are given by D. F. Stein and J. R. Low, Jr., *ibid.* **31**, 362 (1961); J. S. Erickson, *ibid.* **33**, 2499 (1962); A. R. Chaudhuri, J. R. Patel, and L. G. Rubin, *ibid.* **33**, 2736 (1962); and M. N. Kabler, Phys. Rev. **130**, 54 (1963).

[4] J. J. Gilman, Australian J. Phys. **13**, 326 (1960).

[5] V. Celli, M. Kabler, T. Ninomiya, and R. Thomson, Phys. Rev. **130**, 58 (1963).

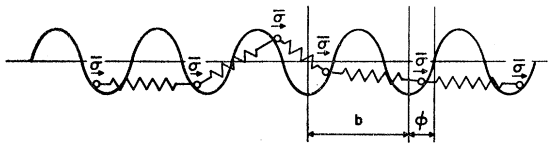

FIG. 1. Modified Frenkel-Kontorova dislocation model. Potential wells and peaks are parabolic. ϕ is distance to change of curvature.

sionless variables will be employed:

$$\sigma=\bar{\sigma}/(k_2 b);\quad P=k_2/k_1$$
$$\gamma=\phi/b;\qquad Q=2\gamma P/(1-2\gamma). \tag{2.2}$$

As in I, an atom in a potential well will be termed subject to a strong bond while an atom on a potential peak will be termed subject to a weak bond. (The terms "well" and "peak" here refer to the entire portion of the potential surface with positive and negative curvature, respectively.) It is shown in I, that for given values of P, γ and $\sigma<\sigma_P$ (the Peierls stress of the model), there exists one stable equilibrium configuration of the model and one unstable equilibrium configuration, the latter having precisely one more weak bond than the former. For simplicity, attention is confined in this paper to values of P and γ such that the stable equilibrium configuration has only one weak bond.

Consider now the dislocation in motion. We make the provisional assumption that the successive configurations of the dislocation are as in Fig. 2, that is, with (1) only one weak-bond atom (the atom $j=0$) in the time interval $\bar{t}_1<\bar{t}<\bar{t}_2$, (2) two weak-bond atoms, $j=0$, 1 in the time interval $\bar{t}_2<\bar{t}<\bar{t}_3$, (3) one weak-bond atom, $j=1$ for $\bar{t}_3<\bar{t}<\bar{t}_4$, etc.

Let $\bar{q}_j^S$ be the atom displacements from their equilibrium positions under zero stress with $j=0$ the only weak-bond atom. (The superscript S emphasizes that these displacements are from a stable equilibrium configuration.) Then the equations of motion which apply for $\bar{t}_1<\bar{t}<\bar{t}_2$ with applied stress $\bar{\sigma}$ are

$$\begin{aligned}&k_1(\bar{q}_{j+1}^S-2\bar{q}_j^S+\bar{q}_{j-1}^S)-k_2\bar{q}_j^S+\bar{\sigma}\\&\qquad=m(d^2\bar{q}_j^S/d\bar{t}^2);\quad |j|>0\\&k_1(\bar{q}_1^S-2\bar{q}_0^S+\bar{q}_{-1}^S)+(2k_2\phi)/(b-2\phi)\bar{q}_0^S+\bar{\sigma}\\&\qquad=m(d^2\bar{q}_0^S/d\bar{t}^2).\end{aligned}\tag{2.3}$$

These may be rewritten in the form

$$d^2q_i^S/dt^2+\sum_j S_{ij}q_j^S=P\sigma;\quad t_1<t<t_2 \tag{2.4}$$

where

$$q_j^S=\bar{q}_j^S/b;\quad t=(k_1/m)^{1/2}\bar{t}, \tag{2.5}$$

and

$$\begin{aligned}&S_{jj}=2+P;\quad |j|>0,\\&S_{00}=2-Q,\\&S_{j,j+1}=S_{j+1,j}=-1;\quad |j|\geqslant 0,\\&S_{ij}=0\quad\text{for}\quad |i-j|>1.\end{aligned}\tag{2.6}$$

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.

Let λ_α^S, $\alpha=0, 1, 2, \cdots$ be the eigenvalues of the matrix $S=[S_{ij}]$ with associated unit eigenvectors $a_{\alpha j}^S$ where the eigenvalues are ordered in increasing magnitude and $a_{\alpha j}^S$ is the displacement of the jth atom in the α mode and let

$$Q_\alpha^S=\sum_j a_{\alpha j}^S q_j^S, \tag{2.7a}$$
$$q_j^S=\sum_\alpha a_{\alpha j}^S Q_\alpha^S. \tag{2.7b}$$

Then the equations (2.4) may be rewritten in the form

$$d^2Q_\alpha^S/dt^2+\lambda_\alpha^S Q^S=P\sigma\sum_i a_{\alpha i}^S;\quad t_1<t<t_2. \tag{2.8}$$

Similar considerations apply for the period $t_2<t<t_3$. We let q_j^U be the (nondimensional) atom displacements from their zero stress (unstable) equilibrium positions, with $j=0$ and $j=1$ the only weak-bond atoms. The equations of motion may then be written in the form analogous to Eq. (2.8) as

$$d^2Q_\alpha^U/dt^2+\lambda_\alpha^U Q_\alpha^U=P\sigma\sum_i a_{\alpha i}^U;\quad t_2<t<t_3, \tag{2.9}$$

where λ_α^U, $a_{\alpha i}^U$ are eigenvalues and associated unit eigenvectors of the matrix $U=[U_{ij}]$ which differs from the matrix S only in the term

$$U_{11}=2-Q, \tag{2.10}$$

and where

$$Q_\alpha^U=\sum_j a_{\alpha j}^U q_j^U, \tag{2.11a}$$
$$q_j^U=\sum_\alpha a_{\alpha j}^U Q_\alpha^U. \tag{2.11b}$$

Local Modes

Because of the modification of the force constants caused by the dislocation, there will be local modes introduced, that is, there will be eigenvectors $a_{\alpha j}$ whose components have appreciable magnitude only in the neighborhood of the dislocation, that is for small $|j|$. Because there is only one weak bond in the time interval $t_1<t<t_2$ one can show by use of Eqs. (2.10) to (2.15a) of I that there will be only one local mode then, a_{0j}^S, corresponding to the minimum eigenvalue λ_0^S. In the time interval $t_2<t<t_3$, when there are two weak bonds,

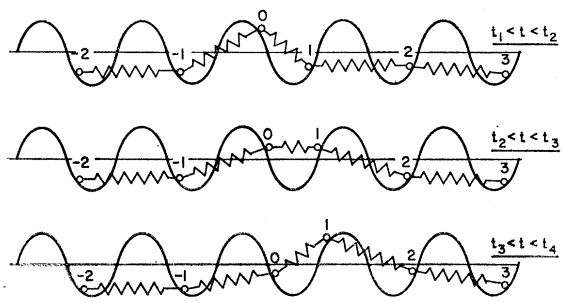

FIG. 2. Assumed sequence of atom positions during dislocation motion.

it can be shown that there will still be only one local mode $a_{0j}{}^U$ corresponding to the minimum eigenvalue $\lambda_0{}^U$, providing P and Q [Eq. (2.2)] satisfy the inequality

$$P+Q\leqslant 2, \tag{2.12}$$

and we restrict attention in this paper to this range of parameters. Furthermore, since the existence of only one weak bond admits (for the range of parameters here considered) a stable equilibrium configuration and two weak-bond atoms admit only an unstable equilibrium configuration, we have $\lambda_0{}^S>0$ and $\lambda_0{}^U<0$.

As has been emphasized recently,[6] the closure property of the eigenvectors of a symmetric matrix implies that when a sharply localized mode exists, all other modes must have small components near the defect. Accordingly, we make here the simplifying assumption that Eqs. (2.7b) and (2.11b) may be approximated for small $|j|$ by

$$q_j{}^S=a_{0j}{}^S Q_0{}^S; \quad t_1\leq t\leq t_2 \tag{2.12a}$$

$$q_j{}^U=a_{0j}{}^U Q_0{}^U; \quad t_2\leq t\leq t_3. \tag{2.12b}$$

These equations can be used to find approximate values of each local normal coordinate (lnc), $Q_0{}^S(t_2)$ and $Q_0{}^U(t_2)$, since at time $t=t_2$, the displacement of the atom $j=1$ is at a distance γ from the point of lowest potential to its left. Therefore, in terms of the equilibrium atom configurations found in I,

$$\begin{aligned} q_1{}^S(t_2)&=\gamma-u_1(0;1),\\ q_1{}^U(t_2)&=\tfrac{1}{2}-\gamma-u_{1/2}(0;1\tfrac{1}{2}), \end{aligned} \tag{2.13}$$

where $u_j(\sigma;M)$ is given by Eq. (2.8) of I.[7] From symmetry considerations we see that the total traverse of each lnc is given by

$$\begin{aligned} d_S&=Q_0{}^S(t_2)-Q_0{}^S(t_1)=2q_1{}^S(t_2)/a_{01}{}^S\\ d_U&=Q_0{}^U(t_3)-Q_0{}^U(t_2)=-2q_1{}^U(t_2)/a_{01}{}^U. \end{aligned} \tag{2.14}$$

Because the atom coordinates $q_j{}^S(t)$ and $q_j{}^U(t)$ differ only in their fixed references, it follows that $\dot{q}_j{}^S(t)=\dot{q}_j{}^U(t)$. The relations between normal coordinate velocities and atom coordinate velocities follow, of course, directly from those between the coordinates themselves, so that in particular from Eq. (2.11a) we get

$$\dot{Q}_0{}^U(t_2)=\textstyle\sum_j a_{0j}{}^U\dot{q}_j{}^U(t_2)=\sum_j a_{0j}{}^U\dot{q}_j{}^S(t_2). \tag{2.15}$$

Since $a_{0j}{}^U$ is a local mode and decays rapidly for large $|j|$, we may get an approximate value for $\dot{Q}_0{}^U(t_2)$ by using in Eq. (2.15) approximate values of $\dot{q}_j{}^S(t_2)$ which are valid for small $|j|$ and which are obtained by differentiation of Eq. (2.12a). This yields the result

$$\dot{Q}_0{}^U(t_2)=\textstyle\sum_j a_{0j}{}^U a_{0j}{}^S\dot{Q}_0{}^S(t_2)=B^{1/2}\dot{Q}_0{}^S(t_2), \tag{2.16}$$

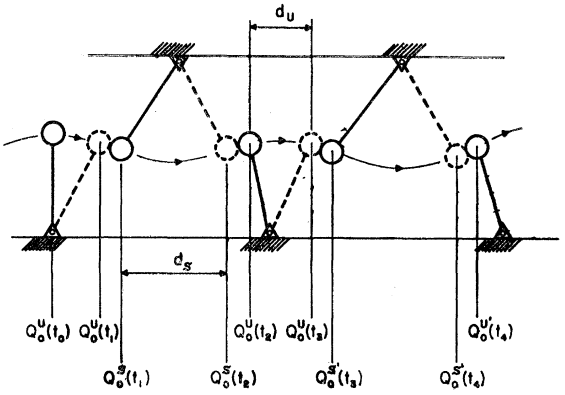

FIG. 3. Pendulum analogy to local normal coordinate motion. The motion of each successive pendulum is regarded as initiated by an inelastic collision [Eqs. (2.16) and (2.17)] with the preceding pendulum.

where, by choosing $a_{0j}{}^U$ and $a_{0j}{}^S$ to be like-oriented unit vectors, we have

$$0<B^{1/2}=\textstyle\sum_j a_{0j}{}^U a_{0j}{}^S<1. \tag{2.16a}$$

Similar considerations apply for the time period $t_3\leq t\leq t_4$ in which the only weak-bond atom is $j=1$. We use superscript S' instead of S to denote all quantities in this time interval. Then, by reasoning completely analogous to the above, we are led to the equation

$$\dot{Q}_0{}^{S'}(t_3)=\textstyle\sum_j a_{0j}{}^{S'}a_{0j}{}^U\dot{Q}_0{}^U(t_3)=B^{1/2}\dot{Q}_0{}^U(t_3), \tag{2.17}$$

where $a_{0j}{}^{S'}=a_{0,j-1}{}^S$, and where the equality

$$\textstyle\sum_j a_{0j}{}^U a_{0j}{}^S=\sum_j a_{0j}{}^{S'}a_{0j}{}^U=B^{1/2}$$

follows from the symmetry properties of $a_{0j}{}^U=a_{0,-j+1}{}^U$, $j\geqslant 1$ and of $a_{0j}{}^S=a_{0,-j}{}^S$.

With the assumptions introduced, we are thus led to the following simple interpretation of the functions $Q_0{}^S(t)$, $Q_0{}^U(t)$, $Q_0{}^{S'}(t)$, etc., as may be seen from their defining equations, (2.8), (2.9), (2.14), (2.16), and (2.17). They describe the motion of a series of alternately suspended (stable) and inverted (unstable) pendulums (Fig. 3) which are each subject to a constant force and each of which transfers energy to its successor only partially. It is this imperfect transfer of energy forward which results in the attainment of a steady dislocation velocity.

Transient and Steady-State Velocities

Consider next successive transfers of energy between local normal modes at times $t_1, t_2, \cdots, t_j, \cdots$ where it is assumed that transfer from a U to a S mode occurs at times t_j, j odd, and that transfer from a S to a U mode occurs at times t_j, j even. Since the motion of each lnc is symmetrical about its zero value, the change in kinetic energy of each lnc during the time interval of its motion is simply the work done on it during that time interval by the effective force acting on it [the right-hand side

[6] R. L. Bjork, Phys. Rev. **105**, 456 (1957). J. A. Krumhansl, J. Appl. Phys. Suppl. **33**, 307 (1962).

[7] It was convenient in I to use a different atomic numbering system depending upon whether $2M$ (the number of weak bonds plus one) was even or odd. With this convention, $u_1(\sigma;1)$ and $u_{1/2}(\sigma;1\frac{1}{2})$, determine the equilibrium positions of the same atom. In this paper, the atomic numbering system is independent of M.

of Eqs. (2.8) or (2.9), respectively, with $\alpha=0$]. Therefore,

$$[\dot{Q}_0{}^S(t_{j+1})]^2-[\dot{Q}_0{}^S(t_j)]^2 = 2P\sigma d_S \sum_i a_{0i}{}^S; \quad j \text{ odd} \tag{2.18}$$

$$[\dot{Q}_0{}^U(t_{j+1})]^2-[\dot{Q}_0{}^S(t_j)]^2 = 2P\sigma d_U \sum_i a_{0i}{}^U; \quad j \text{ even},$$

where d_S, d_U (independent of time) are the total traverses of each of the respective lnc and are given by Eqs. (2.14). To simplify writing, we introduce the notation

$$\begin{aligned} &S_j=[\dot{Q}_0{}^S(t_j)]^2; \qquad U_j=[\dot{Q}_0{}^U(t_j)]^2, \\ &\Delta S=2P\sigma d_S \textstyle\sum_i a_{0i}{}^S; \quad \Delta U=2P\sigma d_U \sum_i a_{0i}{}^U, \end{aligned} \tag{2.19}$$

and rewrite Eqs. (2.18) as

$$\begin{aligned} &S_{j+1}-S_j=\Delta S; \quad j=1, 3, 5, \cdots \\ &U_{j+1}-U_j=\Delta U; \quad j=2, 4, 6, \cdots. \end{aligned} \tag{2.20}$$

Equations (2.16) and (2.17) for the transfer of energy may then be written

$$\begin{aligned} &S_j=BU_j; \quad j=1, 3, 5, \cdots \\ &U_j=BS_j; \quad j=2, 4, 6, \cdots. \end{aligned} \tag{2.21}$$

From Eqs. (2.20) and (2.21) may be derived the following recurrence relations for S_j and U_j:

$$\begin{aligned} &S_{2n+1}-S_{2n-1}=CB^{2n+1}, \quad n\geqslant 1, \\ &U_{2n}-U_{2n-2}=CB^{2n}, \quad n\geqslant 2, \end{aligned} \tag{2.22}$$

where

$$C=(1-B^{-2})U_1+B^{-1}\Delta S+B^{-2}\Delta U. \tag{2.23}$$

These recurrence relations have the solutions

$$\begin{aligned} &S_{2n+1}=S_1+[B^3C(1-B^{2n})]/(1-B^2), \quad n\geqslant 0 \\ &U_{2n+2}=U_2+[B^4C(1-B^{2n})]/(1-B^2), \quad n\geqslant 0. \end{aligned} \tag{2.24}$$

Since $0<B<1$, Eqs. (2.24) lead to steady-state values of S_{2n+1}, V_{2n}, denoted by S_∞, U_∞, respectively. They are

$$\begin{aligned} &S_\infty=[B(\Delta U+B\Delta S)]/(1-B^2); \\ &U_\infty=[B(\Delta S+B\Delta U)]/(1-B^2) \end{aligned} \tag{2.25}$$

and are, as might be expected, independent of the initial value U_1.

In the time interval $t_j\leq t\leq t_{j+1}$, j odd, the lnc $Q_0{}^S(t)$ travels from $Q_0{}^S(t_j)=-\frac{1}{2}d_S$ to $Q_0{}^S(t_j)=\frac{1}{2}d_S$, and its initial velocity $\dot{Q}_0{}^S(t_j)=S_j{}^{1/2}$ is given by Eq. (2.24). The length of the time interval, $t_{j+1}-t_j$, j odd, may therefore be found from the solution of the differential equation governing the motion of $Q_0{}^S(t)$, Eq. (2.8) with $\alpha=0$. The result is

$$\omega_S(t_{j+1}-t_j)=\arcsin\frac{\frac{1}{2}d_S-P\sigma\omega_S{}^{-2}a_S}{[\omega_S{}^{-2}S_j+(\frac{1}{2}d_S+P\sigma\omega_S{}^{-2}a_S)^2]^{1/2}} + \arctan\omega_S S_j{}^{-1/2}(\tfrac{1}{2}d_S+P\sigma\omega_S{}^{-2}a_S); \quad j=1, 3, 5, \cdots, \tag{2.26}$$

where

$$\omega_S{}^2=\lambda_0{}^S; \quad a_S=\textstyle\sum_i a_{0i}{}^S,$$

and principal values of the inverse trigonometric functions are used. Similarly, the length of the time interval $t_{j+1}-t_j$, j even is found to be

$$\omega_U(t_{j+1}-t_j)=\frac{\operatorname{arcsinh}\frac{1}{2}d_U+P\sigma\omega_U{}^{-2}a_U}{[\omega_U{}^{-2}U_j-(P\sigma\omega_U{}^{-2}a_U-\frac{1}{2}d_U)^2]^{1/2}} + \operatorname{arctanh}\omega_U U_j{}^{-1/2}(\tfrac{1}{2}d_U-P\sigma\omega_U{}^{-2}a_U), \tag{2.27}$$

where

$$\omega_U{}^2=-\lambda_0{}^U; \quad a_U=\textstyle\sum_i a_{0i}{}^U.$$

For sufficiently high stress levels and values of j such that $\omega_{S,U}(t_{j+1}-t_j)\ll 1$, the velocity of each lnc is approximately constant throughout the time interval $t_j<t<t_{j+1}$. Under these conditions, the time required for the dislocation to move one atomic spacing $(t_{j+2}-t_j)$ is

$$t_{j+2}-t_j\approx S_j{}^{-1/2}d_S+U_{j+1}{}^{-1/2}d_U; \quad j \text{ odd}$$

and the steady-state dislocation velocity v (normalized with respect to the velocity V_∞ of wave propagation in the linear chain) is approximated for these stress levels by

$$\begin{aligned} v&\approx[S_\infty{}^{-1/2}d_S+U_\infty{}^{-1/2}d_U]^{-1} \\ &\approx\left(\frac{2P\sigma B}{1-B^2}\right)^{1/2}\left[\frac{d_S}{(a_U d_U+Ba_S d_S)^{1/2}}+\frac{d_U}{(a_S d_S+Ba_U d_U)^{1/2}}\right]^{-1}. \end{aligned} \tag{2.28}$$

Dislocation velocity at low stress levels is discussed in the next section.

Dynamic Peierls Stress

The Peierls stress σ_P is the stress required under quasistatic conditions and in the absence of thermal motion to move the dislocation from one stable equilibrium position to an adjacent one. However, once the dislocation is in motion, i.e., has surpassed one potential barrier, it acquires kinetic energy and (at least, for this model) continued motion will be possible at lower stress levels. It appears reasonable to term the minimum stress required to maintain dislocation motion, the dynamic Peierls stress σ_{PD}. This stress is now evaluated.

It is seen from Eq. (2.27) that a finite interval of time $t_{j+1}-t_j$ is possible only if the argument of the arctanh is less than unity or if

$$\sigma>P^{-1}a_U{}^{-1}\omega_U(\tfrac{1}{2}d_U\omega_U-U_j{}^{1/2}), \tag{2.29}$$

i.e., at lower stress levels, the lnc $Q_0{}^U$ with initial velocity $U_j{}^{1/2}$ will not be able to surmount its potential barrier. As seen from Eq. (2.24), U_j approaches its steady-state value, U_∞, monotonically and therefore, independently

of initial conditions, steady-state motion of the dislocation will be possible only if $\sigma>\sigma_{PD}$ where

$$\sigma_{PD}=P^{-1}a_U^{-1}\omega_U(\tfrac{1}{2}d_U\omega_U-U_\infty^{1/2})$$
$$\approx\frac{P^{-1}\omega_U^2d_U^2(1-B^2)}{4[a_Ud_U(1+B^2)+2a_Sd_SB]},\quad(2.30)$$

where the latter form for σ_{PD} is obtained by use of Eq. (2.25) and the fact that $\sigma_{PD}\ll1$. Furthermore, steady motion of the dislocation (in this model) will occur if $\sigma>\sigma_{PD}$ provided only that the process is initiated by a single transfer of energy from a S mode to a U mode. Therefore, in the presence of thermal motion and under an applied stress σ, $\sigma_{PD}<\sigma<\sigma_P$, dislocation motion will begin as soon as thermal motion causes the dislocation to surmount the potential barrier in the direction of the applied stress. It will then continue in motion without further dependence upon thermal motion approaching the steady-state conditions corresponding to S_∞ and U_∞ [Eqs. (2.25)].

Expressions for the eigenvalues and eigenvectors corresponding to the local modes for the modified Frenkel-Kontorova model are given in I [Eqs. (2.12), (2.13), and (2.15a) of I] and from them expressions for the various quantities appearing in Eqs. (2.26) and (2.27) may be derived. The results are

$$\omega_S^2=\lambda_0^S=2+P-[(P+Q)^2+4]^{1/2},$$
$$\omega_U^2=-\lambda_0^U=(Q^2+PQ-P)/(P+Q+1),$$
$$a_S=\left(\frac{1-\bar\beta_S^2}{1+\bar\beta_S^2}\right)^{1/2}\left(\frac{1+\bar\beta_S}{1-\bar\beta_S}\right),$$
$$a_U=\left[\frac{2(1+\bar\beta_U)}{1-\bar\beta_U}\right]^{1/2},\quad(2.31)$$
$$B=\left(\frac{1-\bar\beta_S^2}{1+\bar\beta_S^2}\right)\left(\frac{1-\bar\beta_U^2}{2}\right)\left(\frac{1+\bar\beta_S}{1-\bar\beta_S\bar\beta_U}\right)^2,$$
$$\bar\beta_{S,U}=\tfrac{1}{2}[\bar P_{S,U}+2-(\bar P_{S,U}^2+4\bar P_{S,U})^{1/2}],$$
$$\bar P_{S,U}=P-\lambda_0^{S,U}.$$

Equations (2.26) and (2.27) have been evaluated for the steady-state dislocation velocity v as a function of applied stress σ for $P=0.5$, $\gamma=0.3$ and for $P=1.0$, $\gamma=0.25$. Both exhibited similar behavior and only the former is shown in Fig. 4. These calculations show the very sensitive dependence of velocity upon shear stress at lower stresses which has been observed experimentally.[8] The local mode analysis presented here does not show any upper bound to the dislocation velocity. This question is examined in the next section which describes numerical calculations which do not involve the local mode approximation.

[8] Figure 4 of this paper may be compared with Fig. 5 of Johnston and Gilman, Ref. 3, footnote 3.

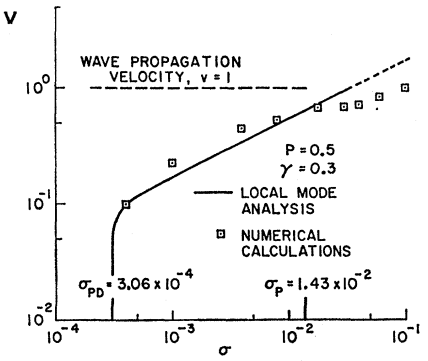

FIG. 4. Stress dependence of steady-state dislocation velocity; comparison of local mode analysis and numerical calculations. A numerical calculation for $\sigma=2.8\times10^{-4}<\sigma_{PD}=3.06\times10^{-4}$ showed that the dislocation failed to surpass the second potential barrier. In terms of the dimensionless variables here employed, $v=1$ corresponds to the speed of wave propagation for infinite wave length in the linear chain with the substrate potential neglected.

3. NUMERICAL CALCULATIONS

In order to check the range of validity of the local mode approximation made in the previous analysis, some numerical calculations were performed on a digital computer. For this purpose, the equations of motion of this model were put in the following finite difference form:

$$x_{j+1}^k-2x_j^k+x_{j-1}^k+F(x_j^k)+P\sigma=(x_j^{k+1}-2x_j^k+x_j^{k-1})(\Delta\tau)^{-2},\quad -N<j<N;\quad k\geqslant1,\quad(3.1)$$

where x_j^k is the (nondimensional) position of the jth atom (measured from the midpoint of the central potential well) at time $t=k\Delta\tau$. The substrate force $F(x_j^k)$ is defined as follows: Let $\xi=x-[x]$, where $[x]$ is the largest (smallest) integer less (greater) than x if x is positive (negative). Then

$$\begin{aligned}F(x)&=-P\xi, && 0\leq|\xi|\leq\gamma\\ &=(\mathrm{sgn}\xi)P(1-|\xi|), && 1-\gamma\leq|\xi|\leq1\\ &=(\mathrm{sgn}\xi)\frac{\gamma P}{1-2\gamma}(2|\xi|-1), && \gamma\leq|\xi|\leq1-\gamma,\end{aligned}\quad(3.2)$$

where $\mathrm{sgn}\xi=+1$ for $\xi>0$, $\mathrm{sgn}\xi=-1$ for $\xi<0$. If we denote by $x_j^k(S)$, the position in the present coordinate system of the jth atom in the (stable) equilibrium configuration under zero stress with $j=0$ the only weak-bond atom, and $x_j^k(U)$ the position of the jth atom in the (unstable) equilibrium configuration under zero stress with $j=0$ and $j=1$ the only weak-bond atoms, then it is seen that

$$x_j^k=x_j^k(S)+q_j^S(t_k);\quad t_1<t_k<t_2,$$
$$x_j^k=x_j^k(U)+q_j^U(t_k);\quad t_2<t_k<t_3,$$

where q_j^S and q_j^U have been defined in Sec. 2. Since $x_j^k(S)$ and $x_j^k(U)$ satisfy Eq. (3.1) with σ and the right-

hand side both equal to zero, it is seen that Eqs. (3.1) and (3.2) are equivalent (except for the finite-difference approximation to the time derivative) to the nondimensional form of Eq. (2.3) and the analogous equation for the period $t_2<t<t_3$. The present form is more convenient for numerical calculations in which the weak-bond atom indices continually change.

The initial conditions were taken to correspond to all the atoms at rest in the (unstable) equilibrium positions under zero stress as computed in I. That is,

$$x_j^0=x_j^1=j+u_{j-1/2} \quad \text{for} \quad j\geqslant 2,$$
$$x_j^0=x_j^1=j+\tfrac{1}{2}+u_{j-1/2} \quad \text{for} \quad j=0,1,$$
$$x_j^0=x_j^1=j+1+u_{j-1/2} \quad \text{for} \quad j\leq -1,$$

where the functions $u_{j-1/2}=u_{j-1/2}\ (0;1\tfrac{1}{2})$ are given by Eqs. (2.8a) of I.[7] The end atoms, $j=\pm N$ were kept fixed. Calculations were performed for the case $P=0.5$, $\gamma=0.3$ with[9] $N=20$ and $\Delta\tau=0.07$. The motion of the dislocation starting from rest until it traveled for 15 lattice spacings was computed at which point, according to the theory of Sec. 2, substantially steady-state conditions are attained. The final velocities are plotted in Fig. 4 and are seen to agree reasonably well with the local mode analysis up to $v\approx 0.7$. Similar agreement was found with numerical calculations for the case $P=1.0$, $\gamma=0.25$. At higher velocities, the number of weak bonds sequence, as observed numerically, changes from 1, 2, 1 to the sequence 1, 0, 1. As the velocity $v=1$ is approached, the dislocation disintegrates with weak-bond atoms appearing at many points throughout the chain and it is then no longer possible to speak of a dislocation velocity.

4. CONCLUSIONS

(1) For the idealized dislocation model considered here, comparison with numerical calculations shows that the local mode approximation describes the dislocation motion fairly well up to dislocation velocities $0.7V_\infty$, where V_∞ is the speed of wave propagation for infinite wavelength in the linear chain with the substrate potential neglected.

(2) The theory indicates that for this model the significant stress parameter is the dynamic Peierls stress, σ_{PD}. For applied stress $\sigma\leqslant\sigma_{PD}$, dislocation motion is possible only with the aid of thermal motion. Dislocation motion will be maintained for any stress $\sigma>\sigma_{PD}$ upon condition that the dislocation has surmounted one potential barrier while the stress is applied, without the further aid of thermal motion.[10] It is found that $\sigma_{PD}\approx 10^{-2}\sigma_P$ for the model parameters here considered.[11]

(3) The model calculations show the extreme stress sensitivity of dislocation velocity at low velocities which has been observed experimentally.

(4) As the velocity V_∞ is approached (at stress levels approximately equal to the static Peierls stress σ_P) the dislocation disintegrates with weak-bond atoms appearing at many points throughout the chain.

It has been noted[12] that under some circumstances, the contribution to the relative atomic displacements near the point of localization of the local mode, of the large number of nonlocal modes, taken together, may be of the same order of magnitude as that of the local mode. The results of the present work appear to indicate that the local modes are nevertheless sufficient to reasonably good approximation for the description of the directed (or athermal) motion of the dislocation. The contribution of the nonlocal modes, it is believed, is of primary importance in the study of thermal effects upon this motion; it is hoped to consider this in a subsequent paper.

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[9] One case, $\sigma=5\times10^{-4}$, was also computed with $N=40$. The results were almost identical to those of $N=20$.

[10] That is to say, the initial conditions used in this paper correspond to the dislocation at the top of the potential barrier with no thermal motion present. In a real crystal under applied stress $\sigma<\sigma_P$, the dislocation could arrive at the top of the barrier only with the aid of thermal motion and the latter would have an effect on the subsequent dislocation motion. This effect has not been studied here.

[11] A discussion of dislocation motion at stress levels below σ_P and another type of explanation is given by D. Kuhlmann-Wilsdorf, Phys. Rev. **120**, 773 (1960).

[12] H. B. Rosenstock and C. C. Klick, Phys. Rev. **119**, 1198 (1960).