Thermal Effects on Dislocation Velocities in a Linear Chain*

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The effects of the thermal motion of atoms upon a dislocation in steady motion in a modified Frenkel-Kontorowa model are examined. The energy associated with the localized mode due to the dislocation and the energy associated with the nonlocalized modes are considered separately and referred to as the energy of the dislocation system and of the surrounding heat bath, respectively. Several distinct components of the net energy exchange between dislocation system and heat bath are isolated. In particular, one component is found which may be described as a coordinating effect between the thermal motion of the atoms and the dislocation motion, which results in a transfer of energy from the heat bath to the moving dislocation. When model parameter values are chosen so that this component of energy transfer is dominant, the drag on a moving dislocation in the model studied decreases with increase in temperature. Computer simulation of the model lends support to the principal features of the theory.

1. INTRODUCTION

BY the employment of a modified Frenkel-Kontorowa model the motion of a dislocation in a linear chain of atoms has been considered in two previous papers.[1,2] In the first, I, the frequency with which a dislocation under an applied stress less than the Peierls' stress σ_P leaves a position of stable equilibrium by means of thermal activation was considered. The second paper, II, dealt with the subsequent motion of the dislocation, once it had surmounted the first potential barrier by thermal activation. It was found in II that sustained steady motion of the dislocation would then be possible without the further intervention of thermal motion if the applied stress exceeded a critical level termed the dynamic Peierls' stress $\sigma_{PD} \sim 10^{-2}\sigma_P$.

It is the purpose of the present paper to use the same dislocation model and to examine the effects of thermal motion upon the sustained dislocation motion which was studied in II from an athermal viewpoint. Previous studies[3] have indicated that the interaction of a moving dislocation with thermal vibrations should result in a drag force on it and consequently a lower steady-state velocity for a given applied stress. For the present simplified model, it is possible to examine the exchange of energy of the dislocation system with the surrounding heat bath[4] of the remaining crystal in greater detail. Several distinct components of the net exchange are isolated. In particular, one component is found which may be described as a coordinating effect between the thermal motion and the dislocation motion. This coordinating effect results in a transfer of energy from the heat bath to the moving dislocation; when this component of energy transfer is dominant, therefore, the effect of the interaction of thermal motion with a moving dislocation is to increase its steady-state velocity for a given applied stress, and the drag on the dislocation decreases with a rise in temperature.

It is, of course, difficult to extrapolate from the behavior of the highly idealized one-dimensional model treated here to the motion of dislocations in real three-dimensional crystals. However, a high degree of idealization is perhaps inevitable in a microscopic or atomistic treatment of such phenomena. One may hope, however, that the analysis of atomistic models may provide insights into the nature of the type of phenomena under study, and that these insights may then prove useful in the construction of models which, being more phenomenological, can include more aspects of reality. For example, a theory for the interpretation of the observed temperature and stress dependence of dislocation velocities in semiconductors has been given by Celli *et al.*[5] This theory, which utilizes the string model of a dislocation, has as essential elements dislocation kinks and dragging points. The nature of dislocation motion in the linear chain of the present paper is obviously a drastic oversimplification of the mode of dislocation motion as described in the model of Celli *et al.* Nevertheless, the results of this analysis may have some relevance to the motion, postulated in that model, of kinks along the dislocation line.

The model employed in the present analysis is described in Sec. 2 and the nature of the coordinating effect is discussed in that and the following section. Anharmonic effects are treated briefly in Sec. 4. Digital-computer simulations of the model were made to verify some aspects of the theoretical analyses. These are described in Sec. 5; conclusions are presented in Sec. 6.

2. MODEL DESCRIPTION AND ANALYSIS

We again consider the modified Frenkel-Kontorowa dislocation model studied in I and II. Only a brief

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

[2] J. H. Weiner, Phys. Rev. **136**, A863 (1964); hereafter referred to as II.

[3] G. Leibfried, Z. Physik **127**, 344 (1950). W. P. Mason, J. Acoust. Soc. Am. **32**, 458 (1960); J. Appl. Phys. **35**, 2779 (1964).

[4] The concepts of energy of the heat bath and of the dislocation refer to energy associated with nonlocalized and localized modes, respectively, and are discussed in greater detail in Sec. 4.

[5] V. Celli, M. Kabler, T. Ninomiya, and R. Thomson, Phys. Rev. **131**, 58 (1963).

description of the model is presented here; for a more complete description and for the notation used but not defined here, the reader is referred to the previous papers.

The model consists of a linear chain of atoms interconnected by linear springs and subjected to a periodic, piecewise quadratic substrate potential (Fig. 1). The horizontal line (hereafter referred to as the transition line) in this figure separates the portions of the potential surface with positive and negative curvature. An atom above this line is referred to as a weak-bond atom; one below, as a strong-bond atom. The parameters P and γ of the model [Eq. (2.2) Ref. 2][6] are chosen, as in II, so that there is only one weak-bond atom ($j=0$) in the stable-equilibrium dislocation configuration under zero stress; the change in energy δE for displacements $q_j{}^S$ of the jth atom from this configuration is given by

$$\delta E=\tfrac{1}{2}\sum_{i,j} S_{ij}q_i{}^S q_j{}^S, \tag{2.1}$$

where the matrix S_{ij} [Eq. (2.6) Ref. 2] is positive-definite. Because of the piecewise quadratic form of the substrate potential, Eq. (2.1) is valid until one of the atoms crosses the transition line. There are two atoms ($j=0, 1$) above the line in the unstable equilibrium position; the corresponding expression for the change in energy from this configuration is

$$\delta E=\tfrac{1}{2}\sum_{i,j} U_{ij}q_i{}^U q_j{}^U, \tag{2.2}$$

where U_{ij} [Eq. (2.10) Ref. 2] has precisely one negative eigenvalue.

It was shown in II that, for appropriate stress levels σ, the dislocation will undergo sustained motion such that (1) in the time interval $t_1<t<t_2$ there will be only one weak-bond atom, $j=0$, (2) in the time interval $t_2<t<t_3$ there will be two weak-bond atoms, $j=0$, 1, (3) in the time interval $t_3<t<t_4$ there will again be only one weak-bond atom, $j=1$, etc.

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

$$Q_\alpha{}^{S,U}=\sum_j a_{\alpha j}{}^{S,U}q_j{}^{S,U} \tag{2.3a}$$

so that

$$q_j{}^{S,U}=\sum_\alpha a_{\alpha j}{}^{S,U}Q_\alpha{}^{S,U}. \tag{2.3b}$$

Because of the presence of the dislocation, $a_{0j}{}^S$ and $a_{0j}{}^U$ are localized normal modes and, as shown in II, a reasonably good approximation to the dislocation motion can be obtained by restricting attention to the motion of the corresponding local normal coordinates (l.n.c.) $Q_0{}^S$ and $Q_0{}^U$. The latter satisfy ordinary differential equations (2.8) (Ref. 2) and (2.9) (Ref. 2) in the time intervals $t_1<t<t_2$ and $t_2<t<t_3$, respectively. We now consider the transition time $t=t_2$.

[6] Equations in I and II are denoted by Ref. 1 and Ref. 2, respectively.

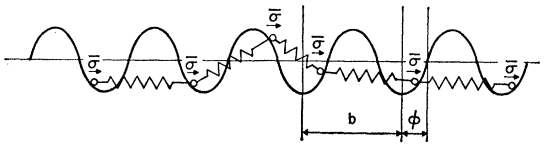

FIG. 1. Modified Frenkel-Kontorowa dislocation model. Potential wells and peaks are parabolic. ϕ is distance to point of change of curvature sign.

Because the atom coordinates $q_j{}^S(t)$ and $q_j{}^U(t)$ differ only in their fixed references, it follows that $\dot{q}_j{}^S(t)=\dot{q}_j{}^U(t)$. We may therefore write

$$\begin{aligned}\dot{Q}_0{}^U(t_2)&=\textstyle\sum_j a_{0j}{}^U\dot{q}_j{}^U(t_2)=\sum_j a_{0j}{}^U\dot{q}_j{}^S(t_2)\\&=\textstyle\sum_{j,\alpha} a_{0j}{}^U a_{\alpha j}{}^S\dot{Q}_\alpha{}^S(t_2)\\&=\textstyle\sum_j a_{0j}{}^U a_{0j}{}^S\dot{Q}_0{}^S(t_2)+\sum_j a_{0j}{}^U\sum_{\alpha\neq 0} a_{\alpha j}{}^S\dot{Q}_\alpha{}^S(t_2)\\&=B^{1/2}\dot{Q}_0{}^S(t_2)+\textstyle\sum_j a_{0j}{}^U\hat{v}_j(t_2),\end{aligned} \tag{2.5}$$

where

$$0<B^{1/2}=\textstyle\sum_j a_{0j}{}^U a_{0j}{}^S<1, \tag{2.6}$$

$$\hat{v}_j(t)=\textstyle\sum_{\alpha\neq 0} a_{\alpha j}{}^S\dot{Q}_\alpha{}^S(t). \tag{2.7}$$

It appears reasonable to refer to $\hat{v}_j(t)$, the portion of the atomic velocity due to all the nonlocalized modes, as the fluctuating component due to thermal motion; while the atomic motion due to the localized mode is considered as that due to the directed dislocation motion. In II, the effects of thermal motion were neglected; that is, the term involving $\hat{v}_j(t)$ was omitted from Eq. (2.5) and the problem solved on that basis. We wish now to examine this aspect of the problem.

If the thermal motion of the atoms corresponds to thermal equilibrium at temperature T, then

$$\langle\hat{v}_j\rangle_t=0, \quad \langle(\hat{v}_j)^2\rangle_t=m^{-1}kT,$$

where the $\langle\ \rangle_t$ denote a time average over a period which is long with respect to the period of thermal vibrations, and m is the atomic mass.

We consider next an ensemble of transitions from a configuration with one weak bond $j=j_W$ to a configuration with two weak bonds $j=j_W$, j_W+1 (briefly an S-to-U transition). This ensemble corresponds to a sequence of many such transitions as the dislocation moves along the chain, so that j_W differs for each transition. It is convenient to introduce, in addition to the fixed atomic index system j, a moving atomic index system $j'=j-j_W$. The atomic thermal velocity will be denoted by $\hat{v}_j$ when the fixed indexing system is used, and by $\hat{w}_{j'}$ when the moving indexing system is used. Thus $\hat{w}_0=\hat{v}_{j_W}$, etc. Let a typical S-to-U transition of the ensemble occur at time t_T. At such time, Eq. (2.5) applies in the form

$$\dot{Q}_0{}^U(t_T)=B^{1/2}\dot{Q}_0{}^S(t_T)+\textstyle\sum_{j'} a_{0j'}{}^U\hat{w}_{j'}(t_T). \tag{2.5'}$$

We average each term of this equation over all of the transitions of the ensemble and denote this average by angular brackets without subscript. The result is

$$\langle \dot{Q}_0{}^U(t_T)\rangle = B^{1/2}\langle \dot{Q}_0{}^S(t_T)\rangle + \sum_{j'} a_{0j'}{}^U \langle \hat{w}_{j'}(t_T)\rangle . \quad (2.8)$$

We note that for a moving dislocation the average $\langle \hat{w}_{j'}(t_T)\rangle$ is one for fixed j' and is thus the average of the thermal velocities at the time of transition of different atoms which are, however, each in the same relative position to the single weak-bond atom before transition. It will also be convenient for some of the discussion to use the notation $\langle \hat{v}_j(t_T)\rangle \equiv \langle \hat{w}_{j'}(t_T)\rangle$ with $j = j' + j_W$. Thus $\langle \hat{v}_{j_W}(t_T)\rangle \equiv \langle \hat{w}_0(t_T)\rangle$, etc. In the absence of any coordinating effect, it may be expected that

$$\langle \hat{v}_j(t_T)\rangle = \langle \hat{v}_j(t)\rangle_t = 0 ,$$

where the equality to zero follows if thermal equilibrium is assumed for the thermal motion. However, for the model under consideration, the time of transition t_T is governed by the motion of a single atom $j = j_T$. For a transition from an S state in which $j = j_W$ is the only weak-bond atom, it is seen that $j_T = j_W + 1$; that is, t_T is the instant when the atom $j = j_T$, $(j' = 1)$ crosses the transition line and changes its bond from strong to weak. In this case it may be expected that a coordinating effect does exist and that therefore

$$\langle \hat{v}_{j_T}(t_T)\rangle \equiv \langle \hat{w}_1(t_T)\rangle \neq 0.$$

If it is assumed[7] that there is no correlation between the thermal velocities of the atoms (which would be the case if the thermal motion corresponded to thermal equilibrium), one would expect $\langle \hat{w}_{j'}(t_T)\rangle = 0$ for $j' \neq 1$. Equation (2.8) then becomes

$$\langle \dot{Q}_0{}^U(t_T)\rangle = B^{1/2}\langle \dot{Q}_0{}^S(t_T)\rangle + a_{01}{}^U \langle \hat{w}_1(t_T)\rangle . \quad (2.9)$$

The average initial velocity $\dot{Q}_0{}^U(t_T)$ of the l.n.c. $Q_0{}^U$ in an S to U transition is therefore due to two separate effects: (1) the "inelastic impact[8]" of the preceding l.n.c. $Q_0{}^S$ and (2) the coordinated thermal effect. It will be shown in the next section, under certain simplifying assumptions, that the coordinated thermal effect is such as to aid the dislocation motion.

For certain model parameter values, discussed in Sec. 5, it is possible that the weak-bond atom $j = j_W$ changes from weak to strong at approximately the same time t_T that the transition atom $j_T = j_W + 1$ changes from strong to weak. In this case we have an S-to-S transition. The changes in the preceding analysis in this case are the expected ones. In particular, Eqs. (2.8) and (2.9) become

$$\langle \dot{Q}_0{}^{S'}(t_T)\rangle = B^{1/2}\langle \dot{Q}_0{}^S(t_T)\rangle + \sum_{j'} a_{0j'}{}^{S'} \langle \hat{w}_{j'}(t_T)\rangle , \quad (2.10)$$

$$\langle \dot{Q}_0{}^{S'}(t_T)\rangle = B^{1/2}\langle \dot{Q}_0{}^S(t_T)\rangle + a_{01}{}^{S'} \langle \hat{w}_1(t_T)\rangle , \quad (2.11)$$

where, as before, $Q_0{}^S$ is the l.n.c. for the state in which $j = j_W$ is the only weak-bond atom, $Q_0{}^{S'}$ is the l.n.c. for the state in which $j = j_W + 1$ is the only weak-bond atom, and $a_{0j}{}^{S'}$ is the corresponding eigenvector. Clearly $a_{0j}{}^{S'} = a_{0,j-1}{}^S$. For this case

$$B^{1/2} = \sum_j a_{0j}{}^S a_{0,j-1}{}^S = 2\beta/(1+\beta^2) , \quad (2.12)$$

where β is defined in Eq. (2.7) (Ref. 1). For future reference, we record here also the value of steady-state dislocation velocity V computed on the athermal basis of II for the S-to-S transition case.

$$V = \left[\frac{P a_S \sigma (1+B^{1/2})}{2 d_S (1-B^{1/2})} \right]^{1/2} , \quad (2.13)$$

where, in addition to the terms previously defined,

$$\begin{aligned} a_S &= [(1-\beta^2)/(1+\beta^2)]^{1/2}[(1+\beta)/(1-\beta)], \\ d_S &= [(2\gamma-\beta)/a_{01}{}^S], \\ a_{0j}{}^S &= [(1-\beta^2)/(1+\beta^2)]^{1/2}\beta^j . \end{aligned} \quad (2.14)$$

3. COORDINATION EFFECT

Consider the motion of the transition atom $q_{j_T}{}^S(t)$:

$$\begin{aligned} \dot{q}_{j_T}{}^S(t) &= a_{0j_T}{}^S \dot{Q}_0{}^S(t) + \sum_{\substack{\alpha \\ \alpha \neq 0}} a_{\alpha j_T}{}^S \dot{Q}_\alpha{}^S(t) \\ &= a_{0j_T}{}^S \dot{Q}_0{}^S(t) + \hat{v}_{j_T}(t) . \end{aligned} \quad (3.1)$$

We consider an ensemble of transition atoms (corresponding conceptually to a sequence of many such transitions) with the assumption that, for fixed but arbitrary t, the ensemble average $\langle \hat{v}_{j_T}(t)\rangle = 0$ so that

$$\langle \dot{q}_{j_T}{}^S(t)\rangle = a_{0j_T}{}^S \langle \dot{Q}_0{}^S(t)\rangle . \quad (3.2)$$

For steady-state dislocation motion, we may regard $\langle \dot{Q}_0{}^S(t)\rangle$ as prescribed; in what follows, we take $\langle \dot{Q}_0{}^S(t)\rangle$ as independent of time. In simpler notation, then, we are concerned with an ensemble of particles each of which starts from the same point at $t = 0$ and moves in the same direction with velocity $v(t;\theta) = a + f(t;\theta)$, where a is a constant and θ is the ensemble parameter taken such that

$$\langle f(t)\rangle = \int_0^1 f(t;\theta)\, d\theta \equiv 0 ; \langle v(t;\theta)\rangle = a . \quad (3.3)$$

Let

$$\xi(t;\theta) = \int_0^t v(\tau;\theta)\, d\tau \quad (3.4)$$

be the distance traveled from the origin, of the member of the ensemble corresponding to θ. Then the transition time $t_T(\theta)$, for this member of the ensemble, is deter-

[7] This assumption is not a critical one because of the strongly localized nature of $a_{0j}{}^U$. It is discussed further in Sec. 5 (particularly Figs. 7 and 8) in the light of a computer simulation of the model.

[8] The term "inelastic impact" is used figuratively with reference to the pendulum model of Ref. 2. It arises from the fact that $B < 1$.

mined implicitly by the equation

$$\xi(t_T(\theta);\theta)=D, \tag{3.5}$$

where D, a constant, is the critical distance. What is desired is $\langle v(t_T(\theta);\theta)\rangle$. In this general form the problem appears difficult to solve. We make here some further simplifying assumptions. First, we assume that

$$v(t;\theta)=a+f(t+\theta), \tag{3.6}$$

so that Eq. (3.5) becomes

$$\int_0^1 f(t+\theta)d\theta=\int_t^{t+1} f(\tau)d\tau=0. \tag{3.7}$$

It follows, in particular, that

$$f(t)=f(t+1). \tag{3.8}$$

The assumption of Eq. (3.6) therefore corresponds to the statement that the random portion of the particle velocity is always the same periodic function, with only the phase being random. Let $V(x;\theta)$ be the velocity of the member of the ensemble corresponding to θ when it reaches the distance x; that is (Fig. 2),

$$V(\xi(t;\theta);\theta)=v(t;\theta). \tag{3.9}$$

Then,

$$\langle v(t_T(\theta);\theta)\rangle=\langle V(D;\theta)\rangle=\int_0^1 V(D;\theta)d\theta.$$

For the ensemble defined by Eq. (3.6),

$$V(D;\theta)=V\left(D+\int_0^\theta v(\tau)d\tau;0\right)=V(D+\xi(\theta)), \tag{3.10}$$

where we have written $\xi(\theta)=\xi(\theta;0)$, $v(\tau)=v(\tau;0)$, and $V(x)=V(x;0)$. Therefore

$$\langle V(D;\theta)\rangle=\int_0^1 V(D+\xi(\theta))d\theta. \tag{3.11}$$

We now use ξ as variable of integration and make use of Eqs. (3.3), (3.4), and (3.8). The result is

$$\langle V(D;\theta)\rangle=\int_0^a \frac{V(D+\xi)}{V(\xi)}d\xi=a+C(D), \tag{3.12}$$

where

$$C(D)=\int_0^a\left[\frac{V(D+\xi)-V(\xi)}{V(\xi)}\right]d\xi \tag{3.13}$$

is the coordination effect on the mean velocity with which particles arrive at the prescribed location D. As a consequence of the velocity periodicity expressed by Eq. (3.8), $V(\xi)$ is also periodic with period a. Therefore, if we choose $n=0,1,2,\cdots$ such that $0\leqslant\eta<a$, where $\eta=D-na$, we may replace D in the integral of Eq. (3.13) by η. We next evaluate this integral for the

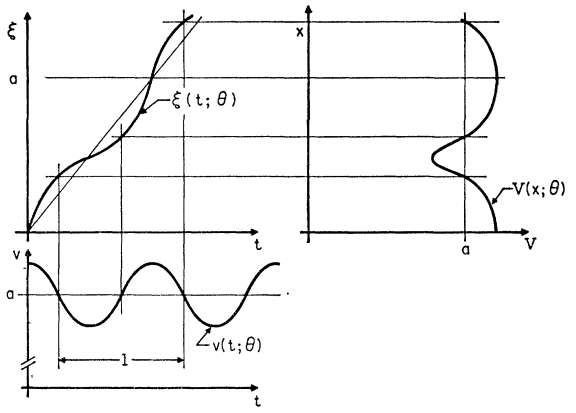

FIG. 2. Illustration for probability discussion of Sec. 3.

piecewise constant velocity,

$$\begin{aligned} v(\theta)&=a-b; \quad 0<\theta<\tfrac{1}{2},\\ &=a+b; \quad \tfrac{1}{2}<\theta<1, \end{aligned} \tag{3.14}$$

with $|b|<a$, a distribution which clearly satisfies Eq. (3.7). Then

$$\begin{aligned} V(\xi)&=a-b; \quad 0<\xi<\tfrac{1}{2}(a-b)\\ &=a+b; \quad \tfrac{1}{2}(a-b)<\xi<a. \end{aligned}$$

Evaluation of the integral leads to the result

$$\begin{aligned} C(\eta)&=\frac{4\eta b}{a^2-b^2}; && 0\leq\eta\leq\tfrac{1}{2}(a-b);\\ C(\eta)&=\frac{2b^2}{a+b}; && \tfrac{1}{2}(a-b)\leq\eta\leq\tfrac{1}{2}(a+b);\\ C(\eta)&=\frac{4(a-\eta)b^2}{a^2-b^2}; && \tfrac{1}{2}(a+b)\leq\eta\leq a. \end{aligned} \tag{3.15}$$

The dependence of the coordination effect upon η is apparently a result of the unrealistic assumption of strict periodicity of all members of the ensemble. In particular, it leads to the result that the increase in the mean velocity due to the coordination effect vanishes for $\eta=0$. However, it is seen that if $b\sim a$, that is, if the fluctuating velocity component is approximately equal in magnitude to the mean velocity, then for almost the entire interval of η,

$$C(\eta)=(2b^2)/(a+b), \tag{3.16}$$

independent of η. It is seen that for $b=a$, the limiting value of b for which the above analysis applies, $C(\eta)\equiv b$; it is clear that $C(\eta)\equiv b$ for $b>a$ as well, for the first crossing of D can then only occur with $v>0$.

4. ANHARMONIC EFFECTS

The discussion has thus far been concerned with a piecewise harmonic linear model. We wish to consider

next the effects of anharmonic terms in such a linear model.

Let, therefore, the potential energy V of the chain be written in the equivalent forms

$$V=\tfrac{1}{2}\sum_{i,j} S_{ij}q_i{}^S q_j{}^S+S_A(q^S) \qquad (4.1S)$$

or

$$V=V_0+\tfrac{1}{2}\sum_{i,j} U_{ij}q_i{}^U q_j{}^U+U_A(q^U), \qquad (4.1U)$$

where the functions $S_A(q^S)$ and $U_A(q^U)$ contain terms of cubic and higher order in the variables $q_i{}^S$, $q_i{}^U$, respectively. The difference in the two forms of the potential-energy function is due solely to the different reference configuration used in measuring the atomic displacements $q_i{}^S$ and $q_i{}^U$. Of course, either form of V may be used for writing the exact equations of motion of the chain for all atom configurations. However, if Eq. (4.1S) is employed, the magnitude of the anharmonic terms $S_A(q^S)$ will increase greatly as the configuration departure from the stable equilibrium position increases, and an analogous statement applies if Eq. (4.1U) is employed. These exact equations of motion may be written in terms of the normal coordinates corresponding to the normal modes of the linearized system in the usual way as either

$$\ddot{Q}_\alpha{}^S+\lambda_\alpha{}^S Q_\alpha{}^S+S_A'(Q^S)=P\sigma\sum_i a_{\alpha i}{}^S \qquad (4.2S)$$

or

$$\ddot{Q}_\alpha{}^U+\lambda_\alpha{}^U Q_\alpha{}^U+U_A'(Q^U)=P\sigma\sum_i a_{\alpha i}{}^U, \qquad (4.2U)$$

depending upon which form of the potential-energy function is used. The functions $S_A'(Q^S)$, $U_A'(Q^U)$ contain terms of quadratic and higher order in the variables $Q_\alpha{}^S$, $Q_\alpha{}^U$, respectively, and introduce coupling among the normal coordinates.

An exact solution of Eqs. (4.2) is neither feasible nor desirable. Rather what is wished is to treat only those of Eqs. (4.2) for which $\alpha=0$, that is for the l.n.c. which describes the directed dislocation motion. Some assumption is then necessary regarding the remaining normal coordinates (usually that their energy distribution corresponds to thermal equilibrium) and the coupling effect treated on some statistical basis. The latter analysis is greatly simplified by an assumption of weak coupling. For example, the work of Toda[9] utilizes this assumption. If an analysis of this type is attempted, therefore, it is necessary to limit the magnitude of the anharmonic terms by utilizing both Eqs. (4.2S) and (4.2U) in appropriate regions.

One means of determining the boundary between these regions is as follows:

Let

$$q_i=q_i{}^S, \quad V_{ij}(q)=[\partial^2 V(q)/\partial q_i\partial q_j],$$
$$V_{ij}(0)=S_{ij}, \quad V_{ij}(d)=U_{ij},$$

where $d=(d_{-N},\cdots,d_N)$ is the displacement of the saddle point from the stable equilibrium configuration. Let $\lambda_0(q)$ be the minimum eigenvalue of the matrix $V_{ij}(q)$, so that $\lambda_0(0)=\lambda_0{}^S>0$ and $\lambda_0(d)=\lambda_0{}^U<0$. For functions $S_A(q)$ and $U_A(q)$ of reasonably restricted nature, we may expect that the coupling terms will be minimized if Eq. (4.2S) is used for q such that $\lambda_0(q)\geqslant 0$ and Eq. (4.2U) is used for q such that $\lambda_0(q)\leqslant 0$. Furthermore, for the case of dislocation motion, only a few of the q_j vary sufficiently to affect the variation of $\lambda_0(q)$ significantly. The results of the piecewise harmonic model suggest that, in fact, the motion of a single atom $j=j_T$ will determine the time t_T at which the change from use of one equation of motion, say Eq. (4.2S), to use of the next form, Eq. (4.2U), takes place. At this transition time, the coordination effect discussed previously in connection with the piecewise harmonic model, should be operative as well in the anharmonic model. In addition, the coupling between modes in the interval between transition times which occurs in the anharmonic model should produce (according to previous analyses such as that of Toda[9]) a drag or energy-loss effect.

Thus, the effect of the interaction of dislocation motion and thermal motion in a linear chain with general potential is separated, from this viewpoint, into two parts: (1) an energy loss due to anharmonic coupling between transition times and (2) an energy gain due to the coordination effect at the transition times. Which of these two terms predominates would seem to depend on the magnitude of the anharmonic terms. If we consider a given state of the dislocation, say an S state, in the time interval $t_1\leqslant t\leqslant t_2$ and refer to the collection of nonlocalized normal modes as the heat bath, then, from the above viewpoint, the energy transfers which occur to and from the dislocation in the S state are shown schematically in Fig. 3.

It should be noted that this separation is not a fundamental one but rather one motivated by the desire for simplified approximate treatment. Should it be possible to solve the statistical interaction problem posed by either Eq. (4.2S) or Eq. (4.2U) for arbitrary interaction functions S_A' or U_A', then such an analysis would require the use of only one of these equations for the entire range of dislocation motion and would yield the net energy gain or loss of the dislocation directly.

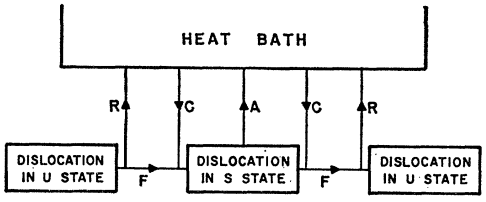

FIG. 3. Schematic of paths of energy flow in dislocation motion. F—Energy transferred forward in inelastic collision. R—Energy rejected upon inelastic collision. C—Energy gain due to coordination effect. A—Energy lost due to anharmonic drag.

[9] M. Toda, J. Phys. Soc. Japan **14**, 722 (1959).

5. COMPUTER SIMULATION

Calculations on a digital computer were undertaken in order to examine the validity of the concept of thermal energy transfer due to the coordinating effect. For this purpose, the piecewise harmonic linear chain model (discussed in I and II) was used in order to eliminate anharmonic drag as far as possible. As we shall see, some anharmonic drag effects are present even in this model in the presence of thermal motion. The reason for this is that the thermal motion produces occasional aberrations in the state sequence of the dislocation; for example, an atom at some distance from the dislocation center may change its bond type during a given state. This results in the coupling of the linear modes corresponding to that state, thus introducing anharmonic drag.

In order to meet the hypotheses of the theory as closely as possible, it was necessary to choose the parameters of the model so that the time required for the dislocation to move one lattice spacing is large compared to the period of vibration of the atoms about their equilibrium sites due to thermal motion. This was accomplished most conveniently by choosing parameter values for which a solution with one weak bond is on the threshold of instability; that is, where the minimum eigenvalue $\lambda_0{}^S$ of the matrix S_{ij} is zero. As may be seen from the analysis of I and II, when this is the case, both the static Peierls stress σ_P and the dynamic Peierls stress σ_{PD} vanish. Because of the latter effect, it is possible to maintain dislocation motion under arbitrarily small applied stress and to choose this stress so that the dislocation velocity has an appropriately small value.[10] For the case in which $\lambda_0{}^S=0$, it may be seen that the total transverse d_U [Eq. (2.14) (Ref. 2)] of the l.n.c. $Q_0{}^U$ also vanishes so that it may be expected that in general the dislocation moves from a state in which there is a single weak-bond atom (jth atom) directly to the state in which the only weak-bond atom is the $(j+1)$th, without the usual intervening state in which there are two weak-bond atoms. In the terminology introduced previously, the transitions which occur for these exceptional values of the parameters are S-to-S transitions.

The numerical procedure followed for the digital computer calculations is that described in II, Sec. 3. However, the atoms were given initial velocities (instead of quiescent initial conditions) as follows:

$$dx_j/dt=(-1)^{j/n}(n)^{1/2}A+Ca_{0j}{}^S \quad \text{for } j/n \text{ an integer or zero,} \qquad (5.1)$$
$$=Ca_{0j}{}^S \text{ for } j/n \text{ not an integer,}$$

where x_j is the position of the jth atom (referred to a lattice spacing of unity) and the nondimensional time t is defined in (2.5) (Ref. 2). The quantity $C(\sigma)$ was chosen so that the initial velocity of the dislocation corresponded to that predicted by the localized mode analysis of II which neglects the effect of thermal motion. The component of the initial velocity alternating in sign was used to simulate thermal motion; the parameter n allows some variation in initial conditions with average initial kinetic energy per atom equal to $\frac{1}{2}A^2$, independent of n.

All the calculations reported on here were performed for parameter values $P=0.5$, $\gamma=\frac{1}{3}$, $\sigma=5\times10^{-4}$, and $N=35$ (so that there were 71 atoms in the chain). In all the runs the computations were continued until the dislocation, starting from the center of the chain, moved twenty lattice spacings under the applied stress. Nine runs were made for various values of A, $0\leqslant A\leqslant 0.04$ with initial conditions corresponding to $n=2$ in Eq. (5.1). To compare the effect of different initial conditions, the case of $A=0.03$ was also run for $n=3$ and $n=4$. For the case of $A=0$ (no initial thermal motion), the digital computations showed, with only very occasional aberrations, that the sequence of states occurred as assumed in the analysis of II and above (that is, S to S). As A was increased, the number of irregularities observed in the state sequence also was increased; this effect was observed as well for the case of $A=0.03$ for the larger values of n. The latter phenomenon is due to the fact that for larger n, fewer atoms are excited, but with proportionately larger initial energy.

The results of the computations are shown in Figs. 4 to 9. In the nondimensional terms used in II, the average dislocation velocity between two successive S-to-S transitions is simply the inverse of the time interval between them. As is to be expected, the energy interchange between dislocation and heat bath varies with each transition and accordingly the dislocation velocity fluctuates, the magnitude of the observed fluctuations being approximately $\pm20\%$. The average dislocation velocity for the total distance of twenty lattice steps traversed is shown in Fig. 4 for the various

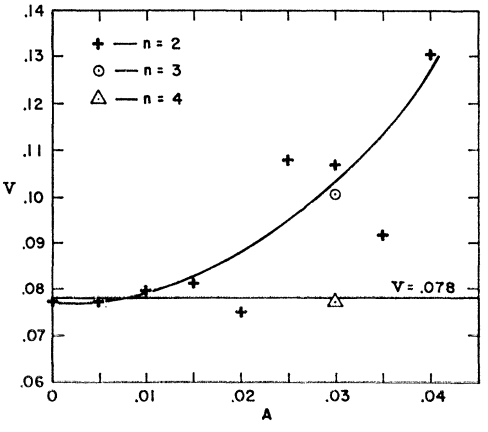

FIG. 4. Average dislocation velocity as determined by computer simulation.

[10] It is also theoretically possible to get very low dislocation velocities by choosing $\sigma-\sigma_{PD}$ small when $\sigma_{PD}>0$. However, in this case the velocity is extremely sensitive to the applied stress σ (see Fig. 4 of II), and this creates computational difficulties.

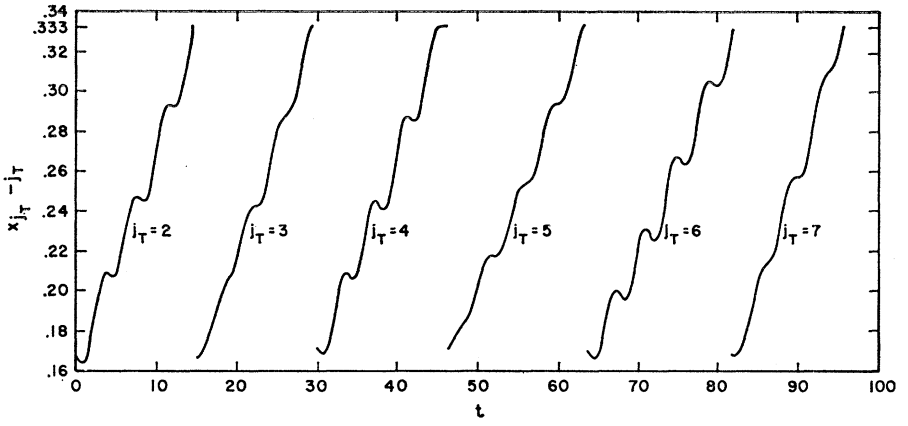

FIG. 5. Typical paths of successive transition atoms, $A=0.01$, $n=2$. $x_{j_T}-j_T$ is distance of transition atom from nearest potential well on its left. Critical distance from this point is $\gamma=\frac{1}{3}$.

values of A. The general trend is seen to be increased steady-state velocity with increase in A, (which corresponds to an increase in temperature), in accordance with the concept of thermal energy transfer to the dislocation due to the coordinating effect. The departures from this trend can be attributed, it is believed, primarily to anharmonic drag effects; this appears to be the case, for example, for the calculations for $A=0.03$, $n=3$ and 4, where the larger amplitude of thermal motion of the fewer excited atoms produces more frequent and severe aberrations in the state sequence. Almost all the velocities determined in the computer calculations, as seen in Fig. 4, lie above the value $V=0.078$ given by Eq. (2.13) which is based on the absence of thermal effects.

As stated previously, the parameter values were chosen to obtain several cycles of thermal fluctuation of the transition atom during a given state configuration. That this was achieved is shown in Fig. 5 in which are plotted typical paths of successive transition atoms. The conditions are seen to conform reasonably well to the hypotheses underlying the probability discussion of Sec. 3. The alternation of the severity of the fluctuations observed in Fig. 5 are due to the persistence of the initial conditions ($n=2$). In order to check the probability formula Eq. (3.16), the computer was programmed to compute the average over all the twenty transitions of the fluctuating component of the velocity of the transition atom at the time of transition, that is, the quantity $\langle \hat{w}_1(t_T)\rangle \equiv \langle \hat{v}_{j_T}(t_T)\rangle$. The value of this average as determined by the computer simulation will be referred to as $\langle \hat{v}_{j_T}\rangle_{\text{calc}}$. This average is compared with the theoretical value $\langle \hat{v}_{j_T}\rangle_{\text{th}}$ as predicted by Eq. [3.16], namely,

$$\langle \hat{v}_{j_T}\rangle_{\text{th}} = (2b^2)/(a+b),$$

where a and b were determined from the computer results by the time averages

$$a = a_{01}{}^S\langle \dot{Q}^S\rangle_t;$$
$$b = \langle \hat{v}_{j_T}{}^2\rangle_t{}^{1/2}.$$

The comparison of $\langle \hat{v}_{j_T}\rangle_{\text{calc}}$ and $\langle \hat{v}_{j_T}\rangle_{\text{th}}$ is shown in Fig. 6. The agreement is reasonably good in view of the numerous simplifying assumptions of Sec. 3.

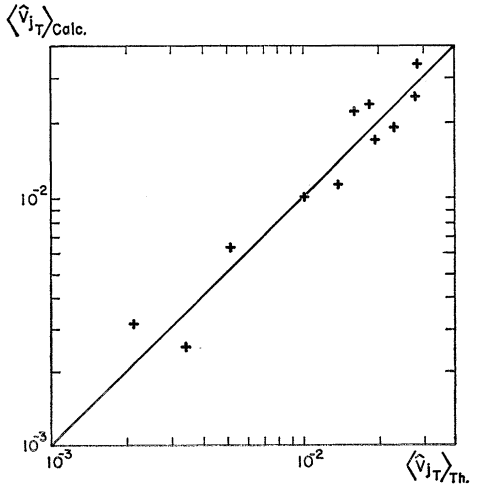

FIG. 6. Comparison of coordination effect as determined by computer simulation $\langle \hat{v}_{j_T}\rangle_{\text{calc}}$ and as given by theory $\langle \hat{v}_{j_T}\rangle_{\text{th}}$.

The next assumption which was examined with the aid of the computer calculations was the degree of correlation between $\hat{v}_j(t_T)$, $j\neq j_T$, and $\hat{v}_{j_T}(t_T)$. In the absence of such correlation, as noted in the discussion leading to Eq. (2.9), one would expect $\langle \hat{v}_j(t_T)\rangle = 0$, $j\neq j_T$, even though the coordinating effect results in $\langle \hat{v}_{j_T}(t_T)\rangle > 0$. In Fig. 7 are plotted $\langle \hat{v}_j(t_T)\rangle$ versus $j-j_T$ as determined from the computer calculations for $A=0.03$ and $n=2$, 3, and 4. It is seen that a high degree of correlation does exist, particularly for the atoms ahead of the dislocation. Here the persistence of the initial conditions is evidenced by the relatively large negative peaks at $j-j_T=2$, 3, and 4 for initial conditions $n=2$, 3, and 4, respectively.

This large correlation between the thermal velocities is probably due to the relatively short time of the computations and the one-dimensionality of the model. As shown by Mazur and Montroll,[11] the rate of correlation decay increases with the dimensionality of the lattice. In spite of the correlation observed in these computations, however, Eq. (2.11) is still a reasonable

[11] P. Mazur and E. Montroll, J. Math. Phys. **1**, 70 (1960).

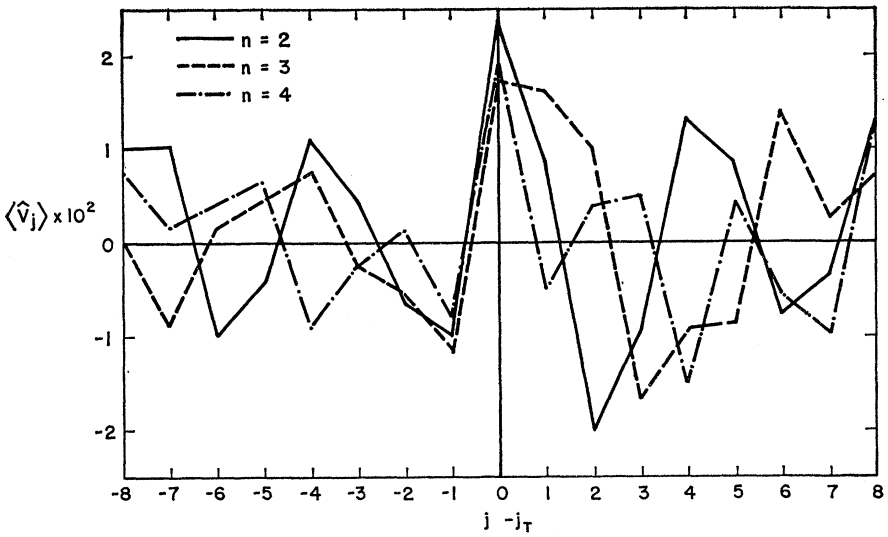

FIG. 7. Computer simulation results. $\langle \hat{v}_j \rangle = \langle \hat{v}_j(t_T) \rangle$.

approximation to the energy transfer due to the coordination effect because of the localized character of the mode $a_{0j}{}^S$. The terms appearing in the sum of Eq. (2.10),

$$a_{0j'}{}^{S'}\langle \hat{v}_{j'}(t_T)\rangle \equiv a_{0,j-j_W}{}^{S'}\langle v_j(t_T)\rangle \equiv a_{0,j-j_T}{}^{S}\langle v_j(t_T)\rangle\,,$$

are shown in Fig. 8 for the case $A=0.03$, $n=2$, and the predominance of the single term of the sum retained in Eq. (2.11) is apparent.

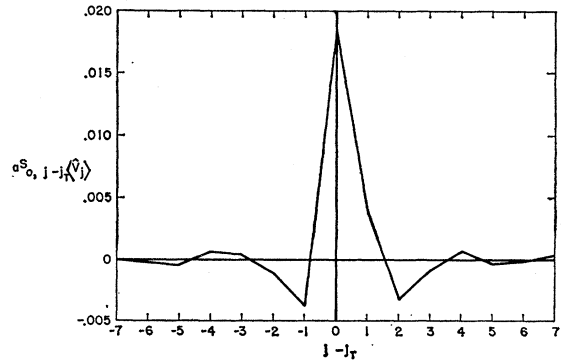

FIG. 8. Computer simulation results, $A=0.03$, $n=2$. $\langle \hat{v}_j \rangle = \langle \hat{v}_j(t_T) \rangle$.

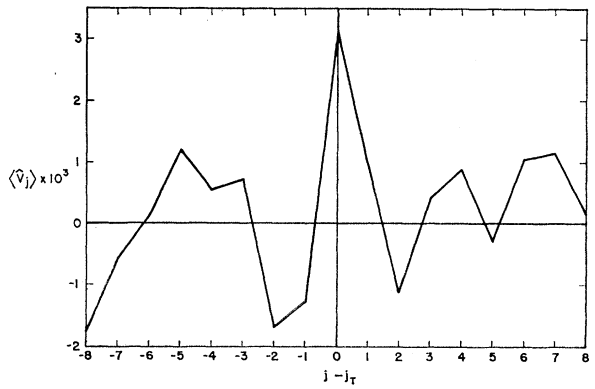

FIG. 9. Computer simulation results, $A=0$. $\langle \hat{v}_j \rangle = \langle \hat{v}_j(t_T) \rangle$.

For the case $A=0$, there is initially no thermal energy in the system. However, as the dislocation moves, thermal energy is transferred to the heat bath because of the inelastic impact effect. The thermal energy which accumulates in the heat bath then is involved in the coordinating effect as well. This is shown in Fig. 9 which is analogous to Fig. 7. As is to be expected, $\langle v_{j_T}(t_T)\rangle$ is much smaller in the case in which $A=0$.

6. CONCLUSIONS

Some conclusions which may be drawn from this work are as follows:

(1) The net interchange of energy of a steadily moving dislocation in the model studied with its surroundings has been separated into a number of distinct components. These are shown schematically in Fig. 3.

(2) In particular, one component is found which may be described as a coordinating effect between atomic thermal motion and dislocation motion. This coordinating effect results in a transfer of thermal energy to the dislocation. When the model parameter values are chosen so that this effect is dominant, therefore, the effect of increased temperature is to increase the steady-state dislocation velocity for a given applied stress.

(3) Digital-computer simulations of the model were made and verified the essential aspects of the theory.

It is believed that a coordinating effect, similar to that described here, may play a role in the motion of other types of defects in solids, and it is hoped that this question may be explored in subsequent work.

ACKNOWLEDGMENTS

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