coming from an ionized phosphorus center weakly coupled to a cluster of two neutral phosphorus atoms.

Note added in proof. Dr. J. J. Pearson made a calculation of J without neglecting the anisotropy of the envelope function. The results will be published in a separate article.

ACKNOWLEDGMENTS

The authors are especially indebted to Professor A. Abragam for very helpful suggestions, and to Dr. Ch. Ryter and Dr. C. Robert for their help on the experimental part of this work.

PHYSICAL REVIEW VOLUME 134, NUMBER 4A 18 MAY 1964

Peierls Stress and Creep of a Linear Chain*

J. H. WEINER AND W. T. SANDERS
Department of Mechanical Engineering, Columbia University, New York, New York
(Received 19 December 1963; revised manuscript received 23 January 1964)

The Frenkel-Kontorova dislocation model is modified by replacing the sinusoidal substrate force by one which is piecewise linear. Exact solutions are found for the static configuration and for the Peierls stress, σ_P. Good agreement is found between these values of σ_P and those obtained previously for a two-dimensional Rosenstock–Newell model. The atoms of the linear chain are then considered in random motion corresponding to thermal equilibrium and under an applied stress $\sigma<\sigma_P$. The time required for motion of the dislocation from one position of stable equilibrium to an adjacent one is computed by means of a rate-theory formulation adapted to the present type of problem in which the positions of all the atoms in the chain are required to vary in passing over the potential barrier. The theoretical transition times for an infinite chain are compared with analog computer results for a six-atom chain and reasonably good agreement is found.

1. INTRODUCTION

THE rate of dislocation creep over the Peierls barrier has been studied in connection both with low-temperature creep[1] and the Bordoni peak.[2] Because of the complexity of the phenomenon, it is necessary to make various assumptions of a mathematical and physical nature when treating a realistic model of the process.

The purpose of the present work has been to construct a simple dislocation model which is amenable to analysis with few additional assumptions. It is hoped that the results of this idealized analysis may provide insight into the nature of the real process, and that the mathematical techniques employed may be applied to more realistic models.

The dislocation model considered here is a modification of the Frenkel-Kontorova one-dimensional model[3] with the sinusoidal substrate force replaced by one which is piecewise linear as in the two-dimensional treatment of Sanders.[4] For this model it is possible to obtain exact solutions to the difference equation describing the static configuration under applied stress and to derive an exact expression for the Peierls stress, σ_P (Sec. 2). The values of σ_P computed here agree surprisingly well with the results of the two-dimensional calculations.[4]

In order to study the dislocation creep rate, the atoms of the model are then considered in random motion corresponding to thermal equilibrium and under an applied stress $\sigma<\sigma_P$. The problem of determining the rate at which the dislocation passes from one stable equilibrium position to an adjacent one is in the general class of problems considered in rate theory.[5] We present here (Sec. 3) a derivation of the pertinent rate formula *ab initio* which is somewhat different from the usual one and is particularly adapted to the present type of problem in which the positions of all the atoms in the chain are required to vary in passing over the potential barrier.

For the infinite chain dislocation model it is possible (Sec. 4) to calculate explicitly all the quantities entering into this rate formula. The theoretically predicted values of the frequency of transition of the dislocation from one equilibrium position to an adjacent one are found to be in order-of-magnitude agreement with analog

* This research was supported jointly by the U. S. Air Force Office of Scientific Research under Grant No. AF-AFOSR-228-63 and by the National Science Foundation under Grant No. NSF-G19010.

[1] J. Lothe and J. P. Hirth, Phys. Rev. **115**, 543 (1959).

[2] A. Seeger, H. Donth, and F. Pfaff, Discussions Faraday Soc. **23**, 19 (1957).

[3] J. Frenkel and T. Kontorova, Phys. Z. Sowjetunion **13**, 1 (1938); J. Phys. (U.S.S.R.) **1**, 137 (1939). A paper which appeared after this manuscript was submitted [J. Kratochvil and V. L. Indenbom, Czech. J. Phys. **13**, 814 (1963)] treats the same modification of the Frenkel-Kontorova model from the static viewpoint only.

[4] W. T. Sanders, Phys. Rev. **128**, 1540 (1962).

[5] H. Eyring, J. Chem. Phys. **3**, 107 (1935); C. Wert and C. Zener, Phys. Rev. **76**, 1169 (1949); C. Wert, *ibid.* **79**, 601 (1950). A paper which came to our attention after this manuscript was submitted is G. H. Vineyard, Phys. Chem. Solids **3**, 121 (1957), which also develops the pertinent rate formula from the viewpoint of Sec. 3. We have retained the present discussion, which differs somewhat in emphasis, for the sake of completeness.

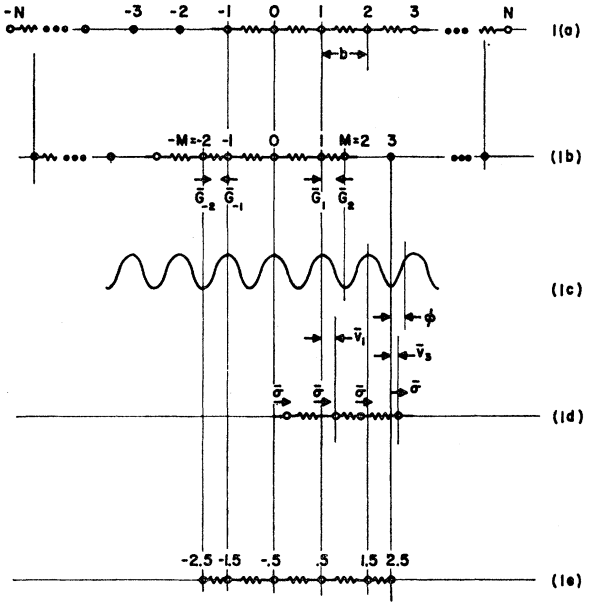

FIG. 1. Linear chain dislocation model.

computer results for a 6-atom chain. Finally, a summary and conclusions are presented in Sec. 5.

2. STATIC SOLUTION

Model Description

As a simplified crystal model, we consider a linear chain of mass points (hereafter referred to as atoms) interconnected by linear springs with spring constant k_1 and equilibrium spacing b (corresponding to the lattice parameter) and subjected also to a periodic (with period b) substrate potential. This substrate potential, as in the original Frenkel-Kontorova model, represents the net effect of the remaining atoms in the (3-dimensional) crystal. We assume a piecewise quadratic, continuous potential $U(x)$, namely,

$$\begin{aligned} U(x)&=\tfrac{1}{2}k_2x^2, && |x|\leq\phi,\\ &=\tfrac{1}{4}k_2\phi b-\frac{k_2\phi}{b-2\phi}\left(\frac{b}{2}-x\right)^2, && \phi\leq|x|\leq\frac{b}{2}, \end{aligned} \tag{2.1}$$

where x is the distance from a potential minimum. This replacement of the trigonometric potential of Frenkel and Kontorova by the piecewise quadratic potential of Eq. (2.2a) simplifies the analysis and introduces the additional parameter ϕ, the distance from a potential minimum to the nearest point at which the potential curvature is discontinuous and becomes negative; ϕ is thus a measure of the hardness of the crystal. The parameter k_2 in Eq. (2.1) is a measure of the shear modulus of the crystal while the parameter k_1 is a measure of the Young's modulus of the crystal.

In order to introduce a dislocation into this model, we start with the linear chain as in Fig. 1(a) and subject the jth atom to a longitudinal force $\bar{G}_j$, where

$$\bar{G}_M=\bar{G}_{-M+1}=-\tfrac{1}{2}k_1b;\quad \bar{G}_{M-1}=\bar{G}_{-M}=\tfrac{1}{2}k_1b;$$
$$\bar{G}_j=0 \quad \text{all other } j. \tag{2.2a}$$

From this, the following equilibrium configuration will result: All atoms $j\geq M$ are displaced $b/2$ to the left, all atoms $j\leq -M$ are displaced $b/2$ to the right, and those for which $-M<j<M$ are undisturbed.[6] To verify that this is indeed an equilibrium configuration, observe that the sum of the forces acting on each atom vanishes. For the special case $M=2$, this new equilibrium configuration is shown in Fig. 1(b). This configuration provides a model for a dislocation because five atoms, viz., -2, -1, 0, 1, and 2, now occupy a region ordinarily occupied by only four atoms.

Now with these forces still applied, the atoms are subjected to the periodic substrate potential defined in Eq. (2.1) and sketched in Fig. 1(c), and which is positioned relative to the configuration of Fig. 1(b) with either a maximum or minimum at the position of all atoms so that it exerts no forces on them in this configuration.

We next apply forces $-\bar{G}_j$ to the configuration of 1(b) and (c), annulling those originally applied, and also apply a constant force $\bar{\sigma}$ (which represents externally applied shear stress) to each atom. Let the resulting displacement of the jth atom from the configuration of 1(b) be $\bar{v}_j$. With the substrate potential of Eq. (2.1), the substrate force on the jth atom is

$$\begin{aligned} &F_j=-k_2\bar{v}_j \quad \text{for} \quad |j|\geq M, \quad \text{providing} \quad |\bar{v}_j|\leq\phi,\\ &F_j=\frac{2k_2\phi}{b-2\phi}\bar{v}_j \quad \text{for} \quad |j|<M,\\ &\qquad\qquad \text{providing} \quad |\bar{v}_j|\leq\left(\frac{b}{2}-\phi\right). \end{aligned} \tag{2.2b}$$

Note that in the first of Eqs. (2.2b) $\bar{v}_j$ is measured from a potential minimum, while in the second of these equations $\bar{v}_j$ is measured from a potential peak. As will be seen subsequently, the value of M is determined for a given set of parameters so that the inequalities on the atom displacements associated with Eq. (2.2b) are satisfied. The final configuration, after forces $-\bar{G}_j$ and $\bar{\sigma}$ are applied is then as shown in Fig. 1(d). The atoms in the range $|j|<M$ will be termed subject to weak bonds to the substrate potential while the others will be referred to as strong bonds. The number of weak bonds, $n_w=2M-1$, may be odd or even. In the latter case, the atoms will be indexed as shown in Fig. 1(e); that is, j is understood to take on the values $\cdots$, $-1\frac{1}{2}$, $-\frac{1}{2}$, $+\frac{1}{2}$,

[6] Only the infinite chain will be considered in detail and therefore the location of the origin may always be taken as the midpoint of the dislocation. The indices j and M in Eq. (2.2a) may be either integers or half-odd integers; see discussion following Eq. (2.2b).

$1\frac{1}{2}, \cdots$ when $2M$ is odd. Therefore in both cases the weak-bond atoms may be taken to correspond to $-M<j<M$ and both cases may be treated together. The equations of equilibrium for the configuration of 1(d) are

$$k_1(\bar{v}_{j+1}+\bar{v}_{j-1}-2\bar{v}_j)-k_2\bar{v}_j-\bar{G}_j+\bar{\sigma}=0\,,\quad |j|\geq M\,,$$

$$k_1(\bar{v}_{j+1}+\bar{v}_{j-1}-2\bar{v}_j)+\frac{2k_2\phi}{b-2\phi}-\bar{v}_j-\bar{G}_j+\bar{\sigma}=0\,,\qquad -M<j<M\,. \tag{2.3}$$

With the introduction of the dimensionless variables

$$\begin{aligned} &v_j=\bar{v}_j/b\,, && G_j=\bar{G}_j/(k_1b)\,;\\ &\sigma=\bar{\sigma}/(k_2b)\,, && P=k_2/k_1\,;\\ &\gamma=\phi/b\,, && Q=\frac{2\gamma P}{1-2\gamma}\,; \end{aligned} \tag{2.4a}$$

and the reduced displacements

$$u_j=v_j-\sigma\,, \tag{2.4b}$$

these equations may be written

$$u_{j+1}-(2+P)u_j+u_{j-1}=G_j\,,\qquad |j|\geq M\,; \tag{2.5a}$$

$$u_{j+1}-(2-Q)u_j+u_{j-1}=G_j-\frac{\sigma P}{(1-2\gamma)}\,,\qquad -M<j<M\,. \tag{2.5b}$$

Displacement Solution

We treat here only the infinite chain, $N\to\infty$; the solutions to Eq. (2.5) which decay at infinity are

$$\begin{aligned} &u_j=A\beta^{-j}\,,\quad j\leq -M\,;\\ &u_j=B\beta^{j}\,,\quad j\geq +M\,;\\ &u_{M-1}=B\beta^{M-1}-\tfrac{1}{2}\,,\quad u_{-M+1}=A\beta^{M-1}+\tfrac{1}{2}\,;\\ &u_j=C\cos j\theta+D\sin j\theta-\frac{\sigma}{2\gamma}\,,\quad -M<j<M\,; \end{aligned} \tag{2.6a}$$

$$u_M=C\cos M\theta+D\sin M\theta-\frac{\sigma}{2\gamma}+\tfrac{1}{2}\,; \tag{2.6b}$$

$$u_{-M}=C\cos M\theta-D\sin M\theta-\frac{\sigma}{2\gamma}-\tfrac{1}{2}\,;$$

where

$$\begin{aligned} &\beta=\tfrac{1}{2}[P+2-(P^2+4P)^{1/2}]\,,\\ &\cos\theta=1-Q/2\,. \end{aligned} \tag{2.7}$$

Equations (2.6a) and (2.6b) satisfy (2.5a) and (2.5b), respectively. The four constants A, B, C, and D may then be determined by the requirement that Eqs. (2.6a) and (2.6b) agree for the four atoms, $-M$, $-M+1$, $M-1$, M for which the expressions overlap. The resulting expressions for the displacements are

$$\begin{aligned} u_j(\sigma;M)&=(\sigma F_M+G_M)\beta^{-j}\,;\quad j\leq -M\,;\\ &=(\sigma F_M-G_M)\beta^{j}\,,\quad j\geq M\,; \end{aligned} \tag{2.8a}$$

$$u_j=\frac{\sigma(\beta-1)\cos j\theta}{2\gamma[\beta\cos(M-1)\theta-\cos M\theta]}+\frac{(\beta-1)\sin j\theta}{2[\sin M\theta-\beta\sin(M-1)\theta]}-\frac{\sigma}{2\gamma}\,,\quad -M<j<M;$$

where

$$\begin{aligned} F_M&=\frac{\cos M\theta-\cos(M-1)\theta}{2\gamma[\beta^M\cos(M-1)\theta-\beta^{M-1}\cos M\theta]}\,,\\ G_M&=\frac{\sin M\theta-\sin(M-1)\theta}{2[\beta^M\sin(M-1)\theta-\beta^{M-1}\sin M\theta]}\,. \end{aligned} \tag{2.8b}$$

In order to complete the solution for the displacements, it is necessary to determine the value of M, characterizing the number of weak bonds, which corresponds to given values of P, the force constant ratio, $\gamma=\phi/b$, and the applied stress, σ. We proceed in an inverse fashion, regarding M as well as P as prescribed, and determine the range of γ for which a solution with $n_w=2M-1$ weak bonds is (1) compatible with the assumed force law (2.2b) and (2) is mechanically stable.

For compatibility, the following conditions are necessary [see Eq. (2.2b)]:

$$\begin{aligned} &\bar{v}_M\leq\phi\,, && \bar{v}_{-M}\geq-\phi\,,\\ &\bar{v}_{M-1}\geq-\left(\frac{b}{2}-\phi\right)\,, && \bar{v}_{-M+1}\leq\left(\frac{b}{2}-\phi\right)\,; \end{aligned} \tag{2.9a}$$

these will later be shown to lead to sufficient conditions. With the use of Eqs. (2.4) and (2.8) these inequalities become

$$\gamma\geq-\beta^MG_M+\sigma(1+\beta^MF_M)\,,\gamma\geq-\beta^MG_M-\sigma(1+\beta^MF_M)\,;$$

and (2.9b)

$$\begin{aligned} &\gamma\leq-\beta^{M-1}G_M+\sigma(1+\beta^{M-1}F_M)\,,\\ &\gamma\leq-\beta^{M-1}G_M-\sigma(1+\beta^{M-1}F_M)\,. \end{aligned}$$

Clearly, if a given bond configuration is not compatible without stress it is not compatible under stress. The stress-free compatibility range is

$$-\beta^MG_M\leq\gamma\leq-\beta^{M-1}G_M\,. \tag{2.9c}$$

Through the use of Eqs. (2.7) and (2.8b) together with some trigonometric manipulation, the following implicit

equation for the lower limit on γ is obtained:

$$\tan M\theta=\frac{1-\beta}{1+\beta}\operatorname{ctn}\frac{\theta}{2}. \tag{2.9d}$$

Let the value of γ^{-1} that satisfies this equation be denoted by C_M. The corresponding equation for the upper limit on γ is

$$\tan(M-1)\theta=\frac{1-\beta}{1+\beta}\operatorname{ctn}\frac{\theta}{2} \tag{2.9e}$$

so that the range corresponding to that of Eq. (2.9c) is

$$C_{M-1}\leq\gamma^{-1}\leq C_M. \tag{2.9f}$$

A detailed investigation shows that some of the inequalities (2.2b) other than those of (2.9a) will be violated unless the lowest values of θ satisfying Eqs. (2.9d) and (2.9e) are chosen. If this is done, then the maximum value of θ in the range (2.9f) satisfies the inequality $(M-1)\theta<\pi/2$, and this can be used together with Eqs. (2.8) to show that for $0<j<M$ u_j is negative and $u_{j+1}<u_j$ and that for $j\geq M$ u_j is positive and $u_{j+1}<u_j$ (only positive j, because of symmetry, need be considered). Then all of the inequalities (2.2) are satisfied.

For the examination of the stability of the equilibrium configuration defined by the displacements u_j it is convenient to return first to the consideration of a finite chain, $-(N+1)\leq j\leq N+1$ [where N may be a half-odd-integer; see Fig. 1(e)] and then to let $N\to\infty$. Let q_j be a small displacement of the jth atom from the equilibrium position being examined, with $q_{-N-1}=q_{N+1}=0$, $V(q_{-N},\cdots,q_N)$ the resulting change in potential energy, and $S_{ij}=(1/k_1)(\partial^2V/\partial q_i\partial q_j)$, $-N\leq i,\ j\leq N$, evaluated at $q_j\equiv 0$. Then

$$\begin{aligned}&S_{jj}=(2+P);\quad -N\leq j\leq -M;\quad M\leq j\leq N;\\ &S_{jj}=(2-Q);\quad -M<j<M;\\ &S_{j,j+1}=S_{j+1,j}=-1;\quad -N+1\leq j\leq N-1;\\ &S_{ij}=0\quad\text{for}\quad |i-j|>1.\end{aligned} \tag{2.10}$$

Let $q(\lambda)=(q_{-N}(\lambda),q_{-N+1}(\lambda),\cdots,q_N(\lambda))$ be an eigenvector of S_{ij} corresponding to the eigenvalue of λ. Then $q_j(\lambda)$ are the solutions to the difference equations

$$\begin{aligned}&q_{j-1}-(2+P-\lambda)q_j+q_{j+1}=0;\\ &\qquad -N\leq j\leq -M;\quad M\leq j\leq N;\\ &q_{j-1}-(2-Q-\lambda)q_j+q_{j+1}=0;\\ &\qquad -M<j<M;\quad q_{-N-1}=q_{N+1}=0.\end{aligned} \tag{2.11}$$

In the terminology of Gantmacher[7] S_{ij} is a normal Jacobi matrix. The eigenvalues λ are then real and simple and are denoted by $\lambda_0<\lambda_1<\cdots\lambda_{2N+1}$. A second property of normal Jacobi matrices is that the sequence $q_{-N}(\lambda_p)$, $q_{-N+1}(\lambda_p)$, $\cdots$, $q_N(\lambda_p)$, $p=0,\ \cdots,\ 2N+1$, has precisely p changes in sign. In order to determine criteria for the positive definiteness of S_{ij} and hence for the stability of a solution with $2M-1$ weak bonds, it is sufficient to consider λ_0 and we therefore seek a solution to Eqs. (2.11) with no changes in sign. This solution, for the case $N\to\infty$ may be written in the form, analogous to that of Eq. (2.6),

$$\begin{aligned}&q_j=A\bar\beta^{-j},\quad j\leq -M+1;\\ &q_j=B\bar\beta^{j},\quad j\geq M-1;\end{aligned} \tag{2.12a}$$

$$q_j=C\cos j\bar\theta+D\sin j\bar\theta,\quad -M\leq j\leq M; \tag{2.12b}$$

where

$$\begin{aligned}&\bar\beta=\tfrac{1}{2}[\bar P+2-(\bar P^2+4\bar P)^{1/2}];\\ &\cos\bar\theta=1-\bar Q/2;\\ &\bar P=P-\lambda,\quad \bar Q=Q+\lambda.\end{aligned} \tag{2.13}$$

The four coefficients, A, B, C, and D are determined by the requirement that Eqs. (2.12a) and (2.12b) agree for the four atoms for which the expressions overlap. The resulting system of four homogeneous equations may be separated into two sets of two each for symmetric and antisymmetric eigenvectors, respectively. We consider only the former set of equations since λ_0 corresponds to a symmetric eigenvector (as noted above, there are no changes in sign in the sequence of its components). They are [with $F=\frac{1}{2}(A+B)$]

$$\begin{aligned}&C\cos M\bar\theta-F\bar\beta^M=0,\\ &C\cos(M-1)\bar\theta-F\bar\beta^{M-1}=0,\end{aligned} \tag{2.14}$$

and equating the determinant of the system to zero leads to the following implicit equation for λ_0,

$$\bar\beta=\frac{\cos M\bar\theta}{\cos(M-1)\bar\theta}, \tag{2.15a}$$

where λ_0 is that root for which $M\bar\theta<(\pi/2)$. We consider next the variation of $\lambda_0=\lambda_0(\gamma^{-1};M)$ with γ^{-1}, with P constant. The following sequence of inequalities may be determined from the equations cited:

$$\frac{d\bar\beta}{d\lambda_0}>0, \qquad [\text{Eq. (2.13)}]$$

$$\frac{d\bar\beta}{d(\cos\bar\theta)}>0. \qquad [\text{Eq. (2.15a)}]$$

Consequently $d(\cos\bar\theta)/d\lambda_0>0$, and from Eqs. (2.4a) and (2.13)

$$\frac{d\gamma^{-1}}{d\lambda_0}=\frac{d\gamma^{-1}}{dQ}\frac{dQ}{d\lambda_0}=-\frac{2P}{Q^2}\left(\frac{dQ}{d\lambda_0}-\frac{1}{2}\right)=\frac{2P}{Q^2}\left[\frac{d(\cos\bar\theta)}{d\lambda_0}+\frac{1}{2}\right]>0.$$

The same result, that a decrease in γ^{-1} decreases λ_0,

[7] F. R. Gantmacher and M. G. Krein, *Oszillationsmatrizen, Oszillationskerne und Kleine Schwingungen Mechanischer Systeme* (Akademie-Verlag, Berlin, 1960), p. 80.

may also be seen directly from Rayleigh's theorems,[8] since, as appears from Eqs. (2.4a), a decrease in γ^{-1} corresponds to an algebraic decrease of the weak-bond spring constants. Therefore the solution corresponding to $2M-1$ weak bonds will be stable only for $\gamma^{-1}\geq S_M$ where S_M is that value of γ^{-1} for which $\lambda_0(S_M; M)=0$. Since for $\lambda_0=0$, $\tilde{\beta}=\beta$ and $\tilde{\theta}=\theta$, the transcendental equation for S_M is

$$\cos M\theta-\beta\cos(M-1)\theta=0, \quad M\theta<(\pi/2); \quad (2.15b)$$

or

$$\tan(M-\tfrac{1}{2})\theta=\frac{1-\beta}{1+\beta}\operatorname{ctn}\frac{\theta}{2}, \quad (2.15c)$$

where Eq. (2.15c) follows upon use of trigonometric identities. Consequently $S_M=C_{M-\frac{1}{2}}$.

Therefore, combining the discussions for compatibility and stability, we may conclude that for a value of γ^{-1} in the range $C_{M-\frac{1}{2}}\leq\gamma^{-1}\leq C_M$ a solution with $2M-1$ weak bonds is both compatible and stable, while the only other compatible solution for the same γ, that with one more weak bond, is unstable.

Peierls Stress

Consider next a linear chain with displacements corresponding to a compatible and stable solution with $2M-1$ weak bonds and apply to it a stress σ which is zero initially and increases slowly (so that inertia effects are negligible). Equations (2.9b) show that this bond configuration will remain compatible while

$$\sigma\leq\frac{\gamma+\beta^M G_M}{1+\beta^M F_M}, \quad \sigma\leq-\frac{\gamma+\beta^{M-1}G_M}{1+\beta^{M-1}F_M}. \quad (2.16a)$$

We define σ_P as the stress above which these inequalities are invalid; for $\sigma>\sigma_P$ the problem has no (statically) compatible solution, i.e., the chain could not support a stress $\sigma>\sigma_P$ in static equilibrium. Therefore σ_P corresponds to the Peierls stress for the model considered. The first of Eqs. (2.16a) may be shown to be controlling; this yields

$$\sigma_P=\gamma\left[\frac{\cos M\theta-\beta\cos(M-1)\theta}{\sin M\theta-\beta\sin(M-1)\theta}\right]\times\left[\frac{\sin M\theta-\delta\sin(M-1)\theta}{\cos M\theta-\delta\cos(M-1)\theta}\right], \quad (2.16b)$$

where $\delta=\beta(2\gamma-1)/(2\gamma-\beta)$. We note that $\sigma_P=0$ for $\gamma^{-1}=C_M$ [this follows from Eq. (2.9d)] and for $\gamma^{-1}=S_M$ [Eq. (2.15b)], that is at the limits of compatibility and stability of configurations with $2M-1$ weak bonds.

Numerical Results

Equation (2.16b) has been evaluated, for values of P (the ratio of noncentral to central forces) equal to 1, 0.5, and 0.2. For each value of P the parameter γ (the ratio of perfect crystal shear strength to shear modulus) was varied over a range wide enough to show the important details of the problem. The results are shown in Figs. 2 and 3; for purposes of comparison Sanders' results,[4] corresponding to $P=0.5$, are also shown in Fig. 2.

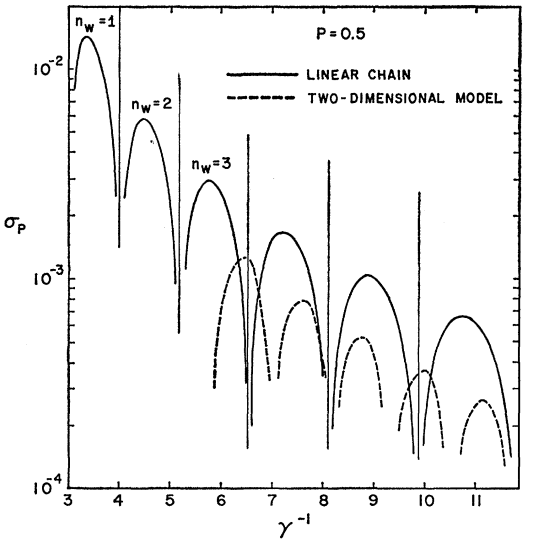

FIG. 2. Peierls stress, σ_P, for linear chain; $P=0.5$. P is the ratio of noncentral to central forces and γ is the normalized critical shear stress of the corresponding perfect crystal. Two-dimensional model results are from Ref. 4.

The agreement between these results and the earlier ones is quite good, in view of the expected sensitivity of the Peierls stress to the details of the model. Both sets have the quasicyclic pattern, and both have about the same exponential dependence on γ^{-1}, while the present results have peak values roughly twice those of the earlier ones.

A qualitative argument would indicate two opposite effects in passing from the one to the two-dimensional model: if the single chain treated here is considered as the first atom row above the slip plane, then the presence of the rows below it would tend to narrow the dislocation, increasing the Peierls stress, while the rows above it would increase the width and lower the stress. Apparently, the latter effect dominates.

The agreement between the one- and two-dimensional cases might serve to substantiate the superiority of the accurate calculation on a discrete model, even a relatively poor model, over the use of a continuum model for dislocation studies.[9]

3. STATISTICAL MECHANICAL CONSIDERATIONS

We wish to consider next the creep, due to thermal motion, of a linear chain, as described in Sec. 2, with a dislocation under an applied stress $\sigma<\sigma_P$. For this

[8] Lord Rayleigh, *The Theory of Sound* (Dover Publications, New York, 1945), Vol. 1, p. 111 *et seq.*

[9] See also R. Hobart and V. Celli, J. Appl. Phys. **33**, 60 (1962).

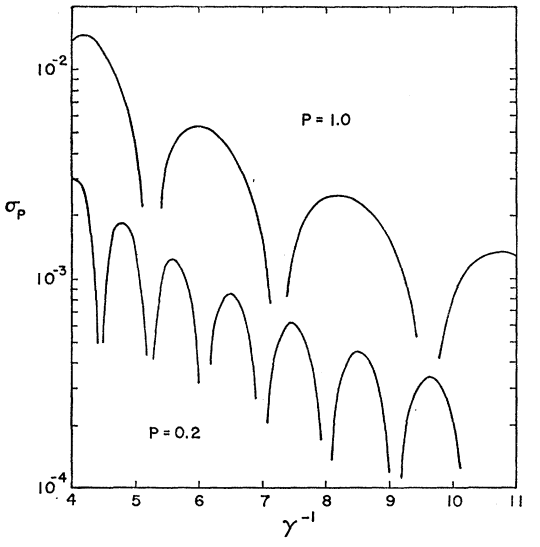

FIG. 3. Peierls stress, σ_P, for $P=1.0$, 0.2.

purpose an ensemble of such chains is assumed with distribution function $\rho(p_{-N},\cdots,p_N,q_{-N},\cdots,q_N)=\rho(p,q)$ where $q_j(t)$ is the displacement at time t of the jth atom from its equilibrium position under stress σ, and $p_j=m\dot{q}_j$ is the momentum of the jth particle with mass m. We treat a chain in thermal equilibrium with its surroundings at temperature T and accordingly set

$$\rho(p,q)=Ce^{-H/kT}, \tag{3.1}$$

where

$$H(p,q)=(1/2m)p_jp_j+V(q_{-N},\cdots,q_N), \tag{3.2}$$

$$C^{-1}=\int_\Omega e^{-H(p,q)/kT}\prod_i dp_i\,dq_i. \tag{3.3}$$

In these equations and in the remainder of this section latin subscripts assume the values $-N,\cdots,N$, where by the latter notation we signify zero included. Greek subscripts assume the values $-N,\cdots,-1,1,\cdots,N$, zero excluded. The symbol Ω denotes the full phase space, $-\infty<p_i<\infty$, $-\infty<q_i<\infty$, and the summation convention is employed.

The potential energy function $V(q)$ for the type of system under consideration admits of a number of positions of stable equilibrium with intermediate positions of unstable equilibrium. Let a typical stable equilibrium position have coordinates $q=(q_{-N},\cdots,q_N)=0$. In a neighborhood of $q=0$, the potential $V(q)$ may be approximated by

$$V(q)=(k_1/2)S_{ij}q_iq_j, \tag{3.4}$$

where the matrix $S=[S_{ij}]$, $S_{ij}=(1/k_1)(\partial^2V(0)/\partial q_i\partial q_j)$, is positive-definite. It is now assumed that the system spends most of the time in this neighborhood of $q=0$, so that $\rho(p,q)$ is very small elsewhere, and that therefore for the purpose of computing the normalization constant C, Eq. (3.3), the approximate expression for $V(q)$, Eq. (3.4), may be used. The result is

$$C=\frac{|S|^{1/2}k_1^{N+\frac{1}{2}}}{(2\pi kT)^{2N+1}m^{N+\frac{1}{2}}}, \tag{3.5}$$

where $|S|$ is the determinant of the matrix S.

Consider next the position of unstable equilibrium at $q=d=(d_{-N},\cdots,d_N)$ nearest to the stable equilibrium position at $q=0$. We confine attention to a neighborhood of the saddle point $q=d$ in which the potential $V(q)$ is adequately represented by its quadratic approximation

$$V(q)=V(d)+(k_1/2)U_{ij}(q_i-d_i)(q_j-d_j), \tag{3.6}$$

where

$$U_{ij}=(1/k_1)(\partial^2V(d)/\partial q_i\partial q_j) \tag{3.6a}$$

so that the equations of motion in that neighborhood take the form

$$m\ddot{q}_i=-k_1U_{ij}(q_j-d_j). \tag{3.7}$$

Let λ_i be the eigenvalues of the matrix $U=[U_{ij}]$ with associated unit eigenvectors a_{ij} and let $\lambda_0<0$ be the minimum eigenvalue with the sign of a_{0j} chosen so that $a_{0j}d_j>0$. It is assumed that λ_0 is the only negative eigenvalue.[10] With the orthogonal change in coordinates

$$Q_i=a_{ij}(q_j-d_j), \tag{3.8}$$

Eq. (3.7) assumes the form, for $Q_0(t)$,

$$\ddot{Q}_0=+s^2Q_0,\quad s^2=-k_1\lambda_0/m, \tag{3.9}$$

with the solution

$$Q_0(t)=\tfrac{1}{2}[Q_0(0)+s^{-1}\dot{Q}_0(0)]e^{st}+\tfrac{1}{2}[Q_0(0)-s^{-1}\dot{Q}_0(0)]e^{-st}. \tag{3.10}$$

Therefore, if at an arbitrary instant of time, $t=0$,

$$Q_0(0)=0 \quad \text{and} \quad \dot{Q}_0(0)>0,$$

then $Q_0(t)$ will increase monotonically, at least as long as Eq. (3.5) applies. Since a_{0j} points away from the stable equilibrium position at $q=0$, this result implies that if the system, in its notion in phase space, reaches the hyperplane $Q_0=0$ with positive velocity, it will not return to its original equilibrium position but continue on towards the next equilibrium position.[11] This hyperplane corresponds therefore to the crest of the ridge between the two valleys. In order to compute the frequency, f, with which the system reaches the hyperplane $Q_0=0$ with $\dot{Q}_0>0$, we introduce, as new coordinates for phase space the Q_i as defined by Eq. (3.8) and the corresponding new momenta $P_i=a_{ij}p_j$. The distribution function in terms of these new variables will be denoted by $\rho(P_0,Q_0,P_\alpha,Q_\alpha)$ where the arguments are separated as shown for future convenience. The

[10] For the case of the linear chain described in Sec. 2, it can be proved that only one negative eigenvalue exists.

[11] This statement is, of course, intended only to apply to short times.

frequency f may now be obtained directly by use of a formula derived by Rice.[12] This formula, which requires the assumption of the ergodic hypothesis for its validity, is in the present case,

$$f=\frac{1}{m}\int_0^\infty P_0 dP_0 \int_{\Omega'} \rho(P_0,0,P_\alpha,Q_\alpha)\prod_\alpha dP_\alpha dQ_\alpha, \quad (3.11)$$

where Ω' is the subspace, $-\infty<P_\alpha<\infty$, $-\infty<Q_\alpha<\infty$. This leads, after the integrations in P_i are performed, to

$$f=\frac{k_1^{N+\frac{1}{2}}|S|^{1/2}}{(2\pi)^{N+1}(kT)^N\sqrt{m}} \times\int_{\Omega''}\exp\left\{\frac{-V(0,Q_\alpha)}{kT}\right\}\prod_\alpha dQ_\alpha, \quad (3.12)$$

where Ω'' is the subspace $-\infty<Q_\alpha<\infty$ and $V(Q_0,Q_\alpha)$ is the function $V(q)$ expressed in terms of the new coordinates Q_i. The assumption is next made that, for the purpose of evaluating the integral in Eq. (3.12), $V(0,Q_\alpha)$ may be evaluated from Eq. (3.6), the expression valid in the neighborhood of the saddle point. Then

$$V(0,Q_\alpha)=V(d)+(k_1/2)\textstyle\sum_\alpha \lambda_\alpha Q_\alpha^2. \quad (3.13)$$

Substitution of this expression into Eq. (3.12) leads to the following expression for f:

$$f=f_0\nu e^{-V(d)/kT} \quad (3.14)$$

where

$$f_0=\frac{1}{2\pi}(k_2/m)^{1/2};\quad \nu=\left(\frac{\lambda_0|S|}{P|U|}\right)^{1/2} \quad (3.14a)$$

and where $|U|=\prod_i\lambda_i$ is the determinant of the matrix U. The quotient of determinants may be written

$$|S||U|^{-1}=|I+S^{-1}D|^{-1}, \quad (3.15)$$

where S^{-1} is the matrix inverse to S, I is the unit matrix and $D=U-S$. In the type of problem considered here the difference matrix, D, will have only a few nonzero elements; in this case, the determinant $|I+S^{-1}D|$ may be expressed in terms of a correspondingly low-order determinant, as will be seen in Sec. 4.

4. CREEP OF LINEAR CHAIN

In this section, the rate formula of Eq. (3.14) is applied to the linear chain described in Sec. 2 under an applied stress $\sigma<\sigma_P$.

Saddle-Point Energy, $V(d)$

In Sec. 3, two approximate expressions for $V(q)$, Eqs. (3.4) and (3.6) were given, the first valid in the neighborhood of the stable equilibrium position, $q=0$, and the second valid in the neighborhood of the unstable equilibrium position, $q=d$. For the model described in Sec. 2, with a piecewise quadratic substrate potential, the two regions of validity (referred to as stable and unstable regions, respectively) have a common boundary B, and the displacements q_i^P corresponding to the Peierls stress σ_P fall on B. Therefore, by use of Eqs. (3.4) and (3.6) to evaluate $V(q^P)$, it is found that

$$V(d)=(k_1/2)S_{ij}q_i^Pq_j^P -(k_1/2)U_{ij}(q_i^P-d_i)(q_j^P-d_j). \quad (4.1)$$

The position $q_i=0$ corresponds to stable equilibrium under an applied stress $\bar\sigma<\bar\sigma_P$ (bars denote dimensional quantities). Since the stress-displacement relation is linear within the stable and unstable region, it follows that

$$\partial V(q^P)/\partial q_i=k_1S_{ij}q_j^P=\bar\sigma_P-\bar\sigma, \quad \text{all } i. \quad (4.2)$$

when the position q^P is regarded as arrived at from the stable position. Similarly, if it is regarded as arrived at from the unstable position at $q=d$, we have

$$\partial V(q^P)/\partial q_i=k_1U_{ij}(q_j^P-d_j)=\bar\sigma_P-\bar\sigma, \quad \text{all } i. \quad (4.3)$$

Substitution from Eqs. (4.2) and (4.3) into Eq. (4.1) yields

$$V(d)=\tfrac{1}{2}(\bar\sigma_P-\bar\sigma)\textstyle\sum_i d_i. \quad (4.4)$$

Because of the linear behavior in both regions, $q_i^P(\bar\sigma)$, the displacements to the common B from the equilibrium positions corresponding to the applied stress, $\bar\sigma$, are given by

$$q_i^P(\bar\sigma)=[(\bar\sigma_P-\bar\sigma)/\bar\sigma_p]q_i^P(0),$$
$$d_i(\bar\sigma)-q_i^P(\bar\sigma)=[(\bar\sigma_P-\bar\sigma)/\bar\sigma_P][d_i(0)-q_i^P(0)],$$

so that

$$d_i(\bar\sigma)[(\bar\sigma_P-\bar\sigma)/\bar\sigma_P]d_i(0). \quad (4.5)$$

Therefore, the energy at the saddle point $d(\bar\sigma)$, corresponding to an applied stress, $\bar\sigma$, is

$$V(d(\bar\sigma))=[(\bar\sigma_P-\bar\sigma)^2/2\bar\sigma_P]\textstyle\sum_i d_i(0). \quad (4.6)$$

Consider $V(d(0))$. Let Δ_j be the displacement of the jth atom when the dislocation moves from the stable equilibrium position at $q=0$ to the next adjacent stable equilibrium position. Then $V(0)=V(\Delta)=0$, and $V(d(0))$ can be computed by considering either displacements from $q=0$ or $q=\Delta$. In both cases Eq. (4.6) applies (with oppositely signed $\bar\sigma_P$) so that

$$V(d(0))=\tfrac{1}{2}\bar\sigma_P\textstyle\sum_i d_i(0)=-\tfrac{1}{2}\bar\sigma_P\sum_i(d_i(0)-\Delta_i)$$

or

$$2\textstyle\sum_i d_i(0)=\sum_i\Delta_i=b, \quad (4.7)$$

where b is the Burger's vector of the dislocation. Substitution into Eq. (4.6) then yields the following formula for the saddle-point energy:

$$v(d(\bar\sigma))=\frac{(\bar\sigma_P-\bar\sigma)^2b}{4\bar\sigma_P}=\frac{(\sigma_P-\sigma)^2}{4\sigma_P}k_2b^2. \quad (4.8)$$

[12] S. O. Rice, Bell Syst. Tech. J. 24, 58 (1945). Reprinted in *Selected Papers on Noise and Stochastic Processes*, edited by N. Wax (Dover Publications, New York, 1954), p. 190.

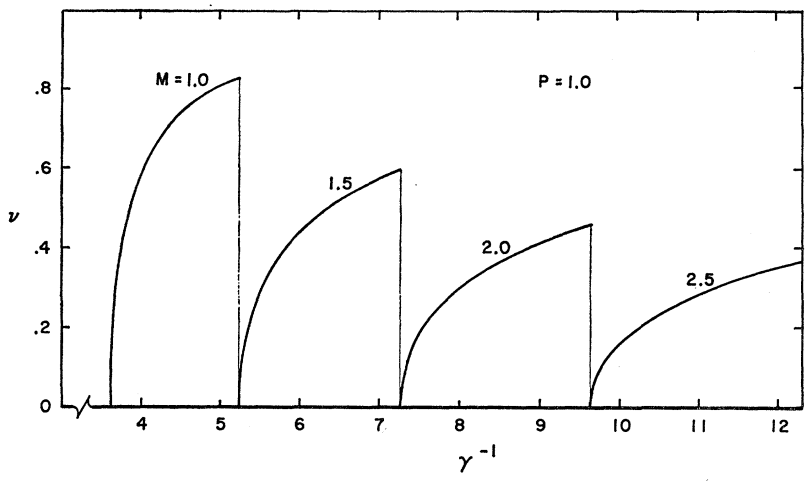

FIG. 4. Variation of the dimensionless frequency ν, Eq. (3.14), with the normalized critical shear stress γ.

Computation of ν

For the model of Sec. 2 which is stable with $2M-1$ weak bonds, only the elements of S and U corresponding to $i=j=M$ differ, so that the only nonzero element of $D=U-S$ is

$$D_{MM}=-(P+Q)=\frac{-P}{1-2\gamma}. \tag{4.9}$$

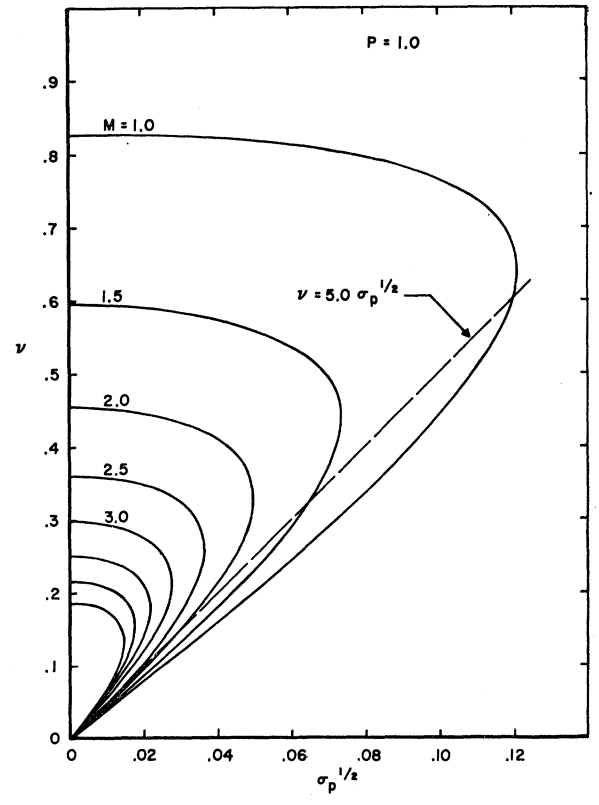

FIG. 5. Variation of the dimensionless frequency ν, Eq. (3.14), with Peierls stress, σ_P.

Substitution in Eq. (3.15) gives the result

$$|S||U|^{-1}=(1+S^{-1}{}_{MM}D_{MM})^{-1} \tag{4.10}$$

so that only the element $S^{-1}{}_{MM}$ of the matrix S^{-1} is needed. This is found (for the infinite chain) by solution of the difference equations $S_{ij}w_j=\delta_{iM}$ with the result

$$S^{-1}{}_{MM}=\frac{\beta}{2}\left[\frac{\cos M\theta}{\cos M\theta-\beta\cos(M-1)\theta}+\frac{\sin M\theta}{\sin M\theta-\beta\sin(M-1)\theta}\right]. \tag{4.11}$$

Finally it is necessary to calculate λ_0, the minimum eigenvalue of the matrix U. This is found from Eq. (2.15a) with M replaced by $M+\frac{1}{2}$. For the case in which stability corresponds to $M=1$, an explicit formula for λ_0 may be derived, namely,

$$\lambda_0=\left[\frac{(2-Q)(P+Q+2)-P-4}{P+Q+1}\right]. \tag{4.12}$$

For other values of M, numerical evaluation of Eq. (2.15a) was used. The resulting values of ν, the dimensionless frequency that appears in the rate equation, Eq. (3.14), are plotted in Fig. 4 for $P=1.0$ as a function of γ. It may be noted that $\nu=0$ for those values of γ which correspond to the limit of stability, S_M, for the given configuration, as does σ_P (Figs. 2 and 3). However, ν increases monotonically within the range $S_M\leq\gamma^{-1}<C_M$, whereas σ_P returns to zero at $\gamma^{-1}=C_M$. It is clear, therefore, that these calculations do not reveal a linear dependence of ν upon $\sqrt{\sigma_P}$ as might be expected from a model treating the dislocation as a single entity moving in a potential field corresponding to σ_P. A plot of ν as a function of $\sqrt{\sigma_P}$, given in Fig. 5, reveals, however, that if only the initial portion of each range of γ is considered, the two quantities are indeed linearly related. It may be that these deviations from

TABLE I. Comparison of theoretical and analog creep rates.

k_2b^2/kT		990	560	245
f/f_0	analog	0.157	0.22	0.46
	theoretical	0.456	0.53	0.595

linearity are due in part to the discontinuous substrate potential employed. If only the initial portions of each range of γ are considered, then the present calculations lead to the relationship $\nu \simeq a\sqrt{\sigma_P}$ with $a=5\pm0.5$ for $0.1\leq P\leq 10$. This may be compared with the similar relationships found, for example, by Seeger,[13] Weertman,[14] and Lothe[1] in their treatments of a dislocation as a vibrating string, the latter two obtaining values of $a=5.6$ and 2.5 respectively.

Analog Computer Results

A REAC Model-400 analog computer was used in an attempt to check these rate calculations, at least in order of magnitude. Because of limitations in equipment only a six-atom model could be simulated; also it was not considered feasible to run through a random sequence of initial conditions, so initial conditions were chosen that would give a minimum frequency of jumps of the dislocation. This model, then, was run for $P=1$, $\gamma=0.2396$, and $\sigma=0.010$ ($\sigma_P=0.0146$), and for three values of temperature. Table I shows these results together with corresponding results based on Eq. (3.14).

The analog data do agree, within a factor of 3, with the theoretical results. The analog results show a lower frequency, as expected (because of initial conditions). They also exhibit a more sensitive dependence on temperature; this again was expected, because of the fact that only six atoms were simulated. In view of the limitations on the analog model, the agreement seems to be good, and appears to lend justification to the assumptions made in the theoretical derivation.

[13] A. Seeger, Phil. Mag. **1**, 651 (1956).
[14] J. Weertman, J. Appl. Phys. **28**, 1185 (1957).

5. CONCLUSIONS

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

(1) The one-dimensional dislocation model yields values for the Peierls stress σ_P in surprisingly good agreement with those for the two-dimensional model considered by Sanders.[4]

(2) In particular, the sensitivity of σ_P to small changes in γ, the critical shear stress, which was found in the two-dimensional calculations[4] is confirmed here.

(3) Detailed results could be obtained on rate of motion of the dislocation under various levels of applied stress less than the Peierls stress and for a range of values of the other parameters of the problem. The relation between these rates and the Peierls stress is in good agreement with that found earlier by treating the dislocation as a vibrating string, except for systematic deviations that are possibly due in part to the discontinuous substrate potential used here.

(4) The rate formula, Eq. (3.14), which has been applied here to a specific one-dimensional model has broader applicability. It allows explicit calculation of rates of transition, without consideration of the concept of entropy of activation, when the potential energy function of the system as a function of the microscopic coordinates is known.

ACKNOWLEDGMENT

The authors wish to thank Mrs. J. H. Clearman who programmed and carried out the numerical calculations.