Calculation of the Peierls barrier with a tension–Frenkel-Kontorova model

Jin-Shown Shie

Institute of Electronics, National Chiao Tung University, Hsinchu, Taiwan, Republic of China

Kuo-Mo Hsiao

Department of Power Mechanical Engineering, National Tsing Hua University, Hsinchu, Taiwan, Republic of China
(Received 13 November 1980)

A tension–Frenkel-Kontorova dislocation model with a nonlinear interatomic force appears to be better justified than previous models in the interpretation of the Peierls stress of dislocation motion. Numerical anisotropic calculations on several fcc crystals result in good agreement within the order of Seeger's double-kink-generation interpretation of Bordoni relaxation peaks. Comparisons of the recalculation results of the Peierls stress with Hobart's compression model suggest that the present tension model is a more realistic representation of an edge-dislocation migration, in which energy is thought to be concentrated on these tension atoms just below the slip plane. It is also possible with this analysis to estimate the surface energies of material studied by internal friction in close agreement. This suggests that the tension–Frenkel-Kontorova model is more than a phenomenological representation of an edge dislocation.

I. INTRODUCTION

The plasticity of solids is caused by dislocation motions in crystals. Owing to the discrete lattice structure, the motion of a dislocation requires on it a minimum shear stress to overcome the Peierls (-Nabarro) barrier.[1,2] Although various continuum approximations, either the original three-dimensional-elasticity methods by Peierls[1] and Nabarro[2] or the one-dimensional Frenkel-Kontorova[3] approximation by Indenbom,[4] have the advantage of using analytical techniques, they also suffer from losing atomistic features, and it becomes difficult to account for the nonlinear interatomic force of crystals. In reality, the core energy might only be a small portion of the dislocation formation energy; however, the core migration energy could be the major contribution to the dislocation migration energy, namely, the Peierls energy. Since atoms in a core are all heavily displaced, the neglect of the nonlinear force effect between these atoms could cause serious errors in evaluating the migration energy. The results were that these continuum approximations gave wider dislocations and therefore smaller barriers for dislocation migration than expected from discrete models.[5,6] This also led some people to question the significance of the Peierls hindering in plastic deformation of solids.[7,8]

Discrete approximations of Peierls barrier calculation have been modeled by many people.[5,6,9-14] Maradudin[9] had considered a three-dimensional lattice of spring-connected atoms in two symmetric configurations (stable and unstable) of a screw dislocation, which allowed him to find the Peierls energy, but not the stress, since the

asymmetric configuration was not available. Hobart[5,10,11] had used the conventional discrete Frenkel-Kontorova model in an exact manner for the analysis of the Peierls barrier, which enabled him to obtain the complete energy variation over a lattice period or Burgers vector. His result[5] for copper had doubled Indenbom's calculation of continuum approximation but was still an order of magnitude less than Seeger's double-kink–generation interpretation[15] on the Bordoni absorption peak[16] of internal friction.[10,17] Recently, Tyson[6] had used a complete two-dimensional atomistic model with two phenomenological interatomic potentials. His numerical calculations gave much higher values of the Peierls stress than that predicted by Peierls and Nabarro. However, owing to the sensitive structure dependence of the Peierls barrier as will be seen below, the use of an equivalent isotropic square lattice to represent an fcc lattice is still a rough approximation which only proves that the discrete calculation will, in general, give higher friction stress.

In the following, we are presenting a tension–Frenkel-Kontorova (TFK) dislocation model. This model[18] (Fig. 2), referred to by Seeger and Schiller as the positive dislocation, has one more substrate-potential valley than the overlaying atoms, so that tension always exists between the atoms. In contrast, the conventional Frenkel-Konotrova (CFK) dislocation model (Fig. 1) always has a compression force existing between the atoms. With linear forces connecting the atoms, the two models are not different from each other in the calculation of the Peierls barrier, but when the nonlinear force is used, the TFK model is found to be overwhelmingly better than the CFK model in the interpretation of an edge-dislocation migra-
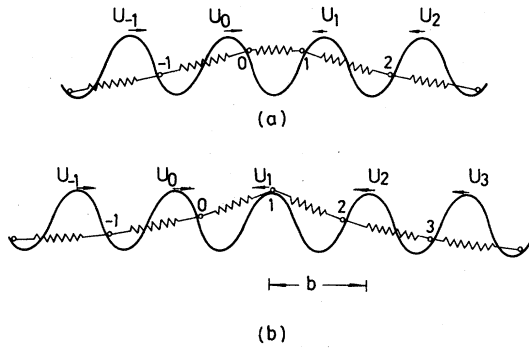
FIG. 1. Configurations of the compression—Frenkel-Kontorova dislocation model: (a) stable, (b) unstable.

tion. We then apply the model to the numerical calculations of the Peierls stress of several widely studied fcc metals, which appear to be close to within an order of magnitude of the values derived from the activation energies of the internal-friction experiments using Seeger's theory of double-kink—generation mechanism. We also reverse the derivations of the analysis, which allows us to estimate from the dislocation—internal-friction data the interatomic forces, and therefore the surface energies of the examined fcc metals along the slip direction. Finally, we discuss the accuracy and the effectiveness of the TFK model.

II. TFK DISLOCATION MODEL

A. Comments on the Frenkel-Kontorova models

Phenomenologically, owing to its simple structure and on account of discreteness, the Frenkel-Kontorova models provide us with simpler and reasonable ways of analyzing the Peierls barrier and with a better chance to obtain analytic solutions, therefore depicting a more physical picture of the dislocation movement.

Figures 1(a) and 1(b) show, respectively, the stable and unstable (saddle-point) configurations
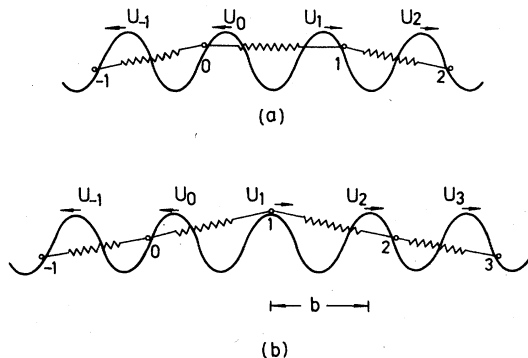

FIG. 2. Configurations of the tension—Frenkel-Kontorova dislocation model: (a) stable, (b) unstable.

of the CFK model. The substrate potential represents the influence of the atoms just below the slip plane to the layer above, which is represented by the spring-connected mass points. Equivalently, their roles are interchangeable, and this TFK model is shown in Figs. 2(a) and 2(b).

When identical linear springs are used for the models,[5] their equations of force equilibrium are both written in the form

$$k(u_{i+1} - 2u_i + u_{i-1}) + \frac{2\pi A}{b} \sin\left(\frac{2\pi u_i}{b}\right) = 0 ,$$
$$i = 0, \pm 1, \pm 2, \ldots$$
(1)

or in the normalized form

$$y_{i+1} - 2y_i + y_{i-1} + P \sin y_i = 0 , \qquad (2)$$

where k is the spring constant between atoms, b the Burgers vector, $P = 4\pi^2 A/kb^2$ the peak value of the normalized substrate potential, and $y_i = 2\pi u_i/b$ the normalized displacement of the ith atom, shown in Figs. 1 and 2 for each model. A is found[5] in the same way as Frenkel[19] did in predicting the theoretical shear strength of a perfect crystal, which reads

$$A = Gb^3c/4\pi^2a \qquad (3)$$

with G the shear modulus and abc the atomic volume. The value of k used by Indenbom[4] and Hobart[5] was found by a plain-strain condition, which is written as

$$k = acE/b(1 - \nu^2) , \qquad (4)$$

where E is Young's modulus and ν is Poisson's ratio. However, owing to the sensitive dependence of the Peierls barrier on the value of P which is a function of A and k, their works[4,5,10,11] of using isotropic values of G and E and the plain-strain condition in finding the spring constant k are very questionable for the following reasons.

(1) Microscopically, the grain in which a dislocation slips is essentially a single crystal, and the use of isotropic elastic constants deviates from reality. As shown in Table I, large differences exist between the isotropic and the directional Young's moduli for the five fcc metals. Hobart mentioned this point in discussing his calculated value.[5] However, with the anisotropic elastic constants of copper put into his model, his result of the Peierls stress worsens to a smaller value due to the smaller P (from 0.47 to 0.3536), as calculated by us in Table II. This is contradictory to his conclusion.

(2) Since grains in a polycrystal solid have no definite shape and orientation, the resultant complicated internal stress distribution around a grain does not justify the use of plain-strain condition in evaluating the spring constant k. The

question remains even in single crystals. In fracture studies, people have used the directional simple-tension condition to evaluate the interatomic force and the bond strength of solids with evident agreement with experiment.[20] Furthermore, judging from internal-friction experiments[21] we think that the simple tension condition is more suitable for evaluating the spring constant k in Frenkel-Kontorova model. As will be derived later, simple tension gives the relationship

$$k = acE/b .$$ (5)

This value is different from that of the plain-strain condition by a factor of $(1 - \nu^2)^{-1}$.

In summary, anisotropic elastic constants and the directional simple-tension derivation of k are believed to be more accurate for the model analysis.

B. Nonlinear interatomic forces

When a nonlinear interatomic force f is introduced, Eq. (1) changes to

$$f(u_{i+1} - u_i) - f(u_i - u_{i-1}) + \frac{2\pi A}{b} \sin\left(\frac{2\pi u_i}{b}\right) = 0 ,$$

$$i = 0, \pm 1, \pm 2, \ldots .$$ (6)

As an illustration, we will use a phenomenological interatomic potential

$$V = -\frac{\alpha}{X} + \frac{\beta}{X^N} ,$$ (7)

where $X = u_{i+1} - u_i + b$ is the distance between atom i and $i+1$. Derive the interatomic forces according to the potential function for Eq. (6) with the conventional CFK model; the result as depicted in Fig. 3 is that the calculated Peierls energy de-
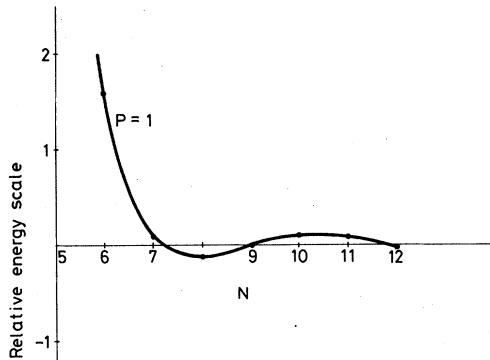
creases with an increase of index N, even to the extent that the stable and the unstable configurations are interchanged as indicated by negative energies. This shows not only that the Peierls barrier is sensitive to the interatomic force form imposed on the model, but also that the effect of the nonlinear repulsive force makes the conventional CFK model unfavorable. The situation does not happen to our TFK model.

In the following analysis, we introduce the sinusoidal interatomic force law as used by Orowan[22] in evaluating the theoretical tensile strength of perfect crystals, which is written

$$f(u_{i+1} - u_i) = f_0 \sin[2\pi(u_{i+1} - u_i)/\lambda] ,$$

$$i = 0, \pm 1, \pm 2, \ldots .$$ (8)

This force law is a good approximation to real crystals in the tension part not exceeding the bond-breaking strength f_0, which is just what we need for our TFK model. The parameters f_0 and λ are related to the surface free energy g_s by

$$f_0 = acE\lambda/2\pi b = ac(Eg_s/b)^{1/2}$$ (9)

and

$$\lambda = 2\pi(g_s b/E)^{1/2} .$$ (10)

Substituting Eqs. (9) and (10) into Eq. (8) and using the small deformation condition, one can readily obtain Eq. (5) discussed above.

C. Numerical solutions

Combining Eqs. (6), (8), (9), and (10), we obtain the force equilibrium conditions in normalized form as

FIG. 3. Difference in energy between the unstable and the stable configurations in compression—Frenkel-Kontorova dislocation model as a function of index N defined in Eq. (7) for a phenomenological interatomic potential. P is the normalized substrate potential defined in Eq. (2).
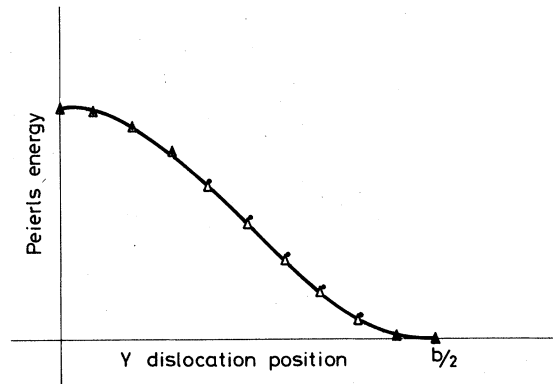

FIG. 4. Calculated Peierls energy by TFK model as a function of dislocation position, Y, defined by Eq. (13). Note that solid line is a sinusoidal curve, dots indicate the values calculated for $P = 0.4126$ and $\Lambda = 1.452$, triangles indicate values for $P = 0.4455$ and $\Lambda = 1.433$.

TABLE I. Crystal parameters of some face-centered cubic metals.

Metal	Elastic moduli at 0 K [a] (10^{12} dyn/cm^2)			Elastic compliances at 0 K [b] (10^{-12} cm^2/dyn)			Elastic constants at 0 K [c] (10^{12} dyn/cm^2)			Burgers vector, $b_{\langle 110\rangle}$ (10^{-8} cm)	Surface energy, g_s (T K) (10^3 erg/cm^2)
	C_{11}	C_{12}	C_{44}	S_{11}	S_{12}	S_{44}	$E_{\langle 110\rangle}$	$G_{\langle 110\rangle}$	E_{iso}		
Cu	1.762	1.249	0.818	1.378	−0.572	1.223	1.411	0.333	1.090	2.56	1.650 [d] (~m.t.)
Ag	1.315	0.973	0.511	2.052	−0.872	1.957	0.927	0.220	0.723	2.89	1.130 [d] (~m.t.)
Au	2.016	1.697	0.454	2.153	−0.983	2.203	0.881	0.204	0.689	2.88	1.350 [d] (~m.t.)
Al	1.143	0.619	0.316	1.412	−0.496	3.165	0.800	0.277	0.687	2.86	1.205 [e] (100 K)
Pb	0.555	0.454	0.194	6.829	−3.073	5.155	0.316	0.067	0.232	3.16	0.442 [e] (623 K)

[a]C. Kittel, in *Phonons*, edited by R. W. H. Stevenson (Oliver and Boyd, London, 1966).
[b]Transformed from elastic moduli of column 2.
[c]Calculated from elastic compliances of column 3 by simple tension condition.
[d]Reference 20.
[e]Reference 23.

$$\sin\left(\frac{y_{i+1}-y_i}{\Lambda}\right) - \sin\left(\frac{y_i-y_{i-1}}{\Lambda}\right) + \frac{P}{\Lambda}\sin y_i = 0,$$

$$i = 0, \pm 1, \pm 2, \ldots \ , \tag{11}$$

where $\Lambda = \lambda/b = 2\pi(g_s/bE)^{1/2}$ is referred to as the maximum strain parameter. In principle, the value of each y_i can be solved according to Eq. (11) for a specified value of y_1 of the largest displaced atom. Denoting y_i as $g_i(y_1)$, the normalized dislocation energy is read as

$$E_d(y_1) = \sum_{i=-\infty}^{\infty} \left(\frac{\Lambda}{2\pi}\right)^2 \left[1 - \cos\left(\frac{g_{i+1}-g_i}{\Lambda}\right)\right.$$
$$\left. + \frac{P}{4\pi^2}(1+\cos g_i)\right]. \tag{12}$$

The Peierls energy E_p is the maximum fluctuation of E_d.

If we define the dislocation position Y to be proportional to y_1 in the first half of the migrational period, that is,

$$y_1 - y_1^{\min} = \frac{y_1^{\max} - y_1^{\min}}{b/2}\ Y, \tag{13}$$

then the Peierls stress σ_p can be obtained as

$$\sigma_p = \frac{2k}{c}\ (y_1^{\max} - y_1^{\min})\frac{dE_d(y_1)}{dy_1}\bigg|_{\max}. \tag{14}$$

In Fig. 4, one can see that the plots of E_p as a function of y deviate little from a sinusoidal curve. This justifies our definition of Y by Eq. (13). The nonlinear force effect makes Hobart's definition difficult to be applied in our model. Although the two definitions are not comparable, they should not differ much from each other in evaluating σ_p. The nonlinear tension releases atom 1 more towards the potential valley; thus it contributes more to the Burgers vector and makes Eq. (13) more effective. The accurate σ_p can also be calculated by Hobart's method[5] of obtaining the maximum force required to pull atom 1 statically while other atoms follow their respective equilib-

TABLE II. Comparisons of Peierls energy and stress for fcc metals under simple tension condition by our TFK model, Hobart's model, and the experiment.

Material	P	$\Lambda/2$	Normalized Peierls energy (10^{-4}) TFK	Hobart's	Peierls stress σ_p ($10^{-4}\ G_{\langle 110\rangle}$) TFK	Hobart's	Experiment [a]
Cu	0.3536	0.671	0.313	0.0088	3.374	0.096	5.03 [b]
Ag	0.3556	0.645	0.468	0.0092	5.008	0.099 [c]	6.22 [b]
Au	0.3464	0.724	0.149	0.0075	1.647	0.082 [c]	11.06 [b]
Al	0.5206	0.721	4.773	0.1510	34.600	1.116 [c]	23.49 [b]
Pb	0.3184	0.628	0.212	0.0037	2.536	0.044 [c]	5.16 [d]

[a]From dislocation–internal-friction experiment, interpreted by Seeger's double-kink–generation theory.
[b]Reference 21. Corresponding activation energies are for Cu, 0.122 eV, Ag, 0.124 eV, Au, 0.158 eV, and Al, 0.25 eV.
[c]Calculated by the authors according to Hobart's original model.
[d]Reference 15. Selected from low-frequency values only.

TABLE III. Calculated Peierls energies and stresses for fcc metals under plain-strain condition by our TFK model and Hobart's model.

Material	P	$\Lambda/2$	Normalized Peierls energy (10^{-5})		Peierls stress σ_p $(10^{-4} \, G_{\langle 110 \rangle})$	
			TFK	Hobart's	TFK	Hobart's
Cu	0.268	0.671	0.233	0.0077	0.332	0.0111
Ag	0.264	0.645	0.269	0.0067	0.389	0.0097
Au	0.235	0.724	0.038	0.0021	0.061	0.0035
Al	0.450	0.690	20.516	0.5670	17.265	0.4820
Pb	0.210	0.628	0.029	0.0006	0.054	0.0012

rium positions.

In the numerical calculations, we first find $y_1^{max} - y_1^{min}$ according to Eqs. (11) and (12). The distance between them is then divided into 20 positions. E_p and σ_p are calculated accordingly at these positions.

III. RESULTS

Table I lists the various numerical values of crystal parameters of five fcc metals required in our analysis. Since the slip direction is along $\langle 110 \rangle$ for the fcc crystal, $G_{\langle 110 \rangle}$ and $E_{\langle 110 \rangle}$ are derived by suitable transformations from values of elastic compliance in the second column of the table under simple tension condition. For the purpose of comparison, as discussed in Sec. II A, the isotropic Young's modulus, E_{iso}, used by previous models is also listed for each metals. Owing to the low-temperature flattening of elastic constants, their values at absolute zero are used as approximations of various low-temperature values with which the internal-friction experiments to be compared were performed. With the exception of aluminum, the surface energies of the other four metals employ their high-temperature values. This is because of many difficulties of obtaining the accurate surface entropies from scarce sources; hence the extrapolation to the low-temperature regime is either unavailable or unreliable. Besides, the configuration around a dislocation differs from that of the surface; therefore the surface-entropy correction might not be meaningful to our dislocation problem. The value for aluminum is extrapolated to 100 K from data given by Bondi.[23] The reason is that the high-temperature value listed in other sources is found too small to "bond" the two central atoms; therefore it makes the calculation unrealistic if a high-temperature value is used. In addition to these uncertainties, we wish to remind the reader here that the surface energies are isotropic values, although the quantities are only weakly directionally dependent for fcc metals.[24,25]

Values of the normalized substrate potential P and the maximum strain parameter Λ are calculated and listed in Table II according to their appropriate definitions. The numerical results of the Peierls energy and stress are listed in the fourth and sixth columns of the table. It is evident that
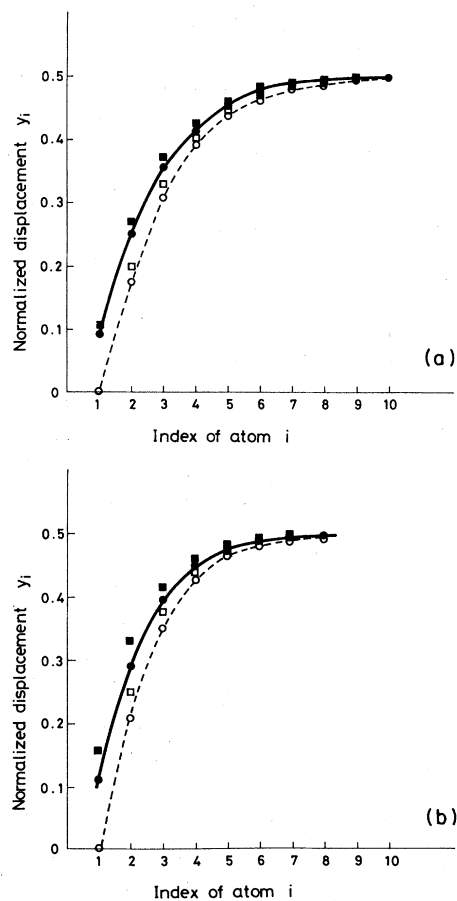

FIG. 5. Normalized displacements of core atoms: (a) gold, (b) aluminum. Circles on lines are the continuum approximations. Squares are our solutions. Note that Al has the largest deviation from the continuum solution while Au has the least in our five illustrated crystals.

the calculated Peierls stresses of the five fcc metals are all within an order of magnitude of the experimental values derived according to Seeger's theory[15] in the interpretation of the Bordoni absorption peak in the internal-friction experiments. The values of the activation energy employed by the double-kink–generation theory here are not those given in Seeger's original paper, but are those discussed by Niblett,[21] which are thought to be more reliable. Listed in the table are also the Peierls energies and stresses calculated according to Hobart's compression model. They are in poor agreement with Seeger's interpretation values. One might wonder if these are due to the prejudice of the simple tension condition applied in the model. Table III lists the calculated values of the Peierls barrier according to the plain-strain condition for these nonisotropic crystals. The results still show that our TFK model is better than the conventional CFK model as used by Hobart, although both are not in accord with experiment, with the exception of our calculated value of aluminum.

IV. DISCUSSIONS

From our analysis discussed above, the movement of an edge dislocation can be interpreted better by the TFK model as supported by our calculated results of fcc metals. Except for Au, most of our calculated values are different from the experimental data by not more than a factor of 2, which had never been done previously.

This suggests that our model is probably close to the true situation of the edge-dislocation migration, where the energy of migration is concentrated on the core atoms just below the slip plane where tension exists. Figures 5(a) and 5(b) illustrate the displacements of core atoms of Au and Al, which are the two extremes of our calculation. It is clear that the tension model gives larger displacements and the atoms relax faster to the potential valleys than does the continuum model. In contrast, the repulsive nonlinearity of the interatomic force makes the CFK model, which has been used in previous work, unfavorable in the evaluation of the Peierls barrier. Tension tries to localize the strain of an edge dislocation around its core region, and therefore traps the dislocation more in its stable configuration. This not only is energetically favorable but also increases the difficulty of escaping to the neighbor stable positions and hence gives a larger barrier energy. In the quasistatic problem, dislocations are required to populate for a longer period of time in the stable configuration than in the unstable. It seems then the principle just implied in the above statement

should be applicable; that is, to test the correctness of the model of the Peierls-barrier calculation requires us to see if the stable configuration is the true ground state. This principle is not applicable to the dynamic problem, where equilibrium of the stable configuration cannot be established in time; therefore a reduction in the Peierls barrier can be expected.[14]

The extreme sensitivity of the Peierls barrier to the value of P also indicates that the isotropic models are very questionable in the precise calculation of the barrier, although they could sometimes describe more qualitative pictures owing to the possibility of using analytic techniques. Nevertheless, they could also lead to incorrect concepts due to the underestimation of the Peierls barrier.

The discrepancies of our results with the experimental data might arise from the following sources.
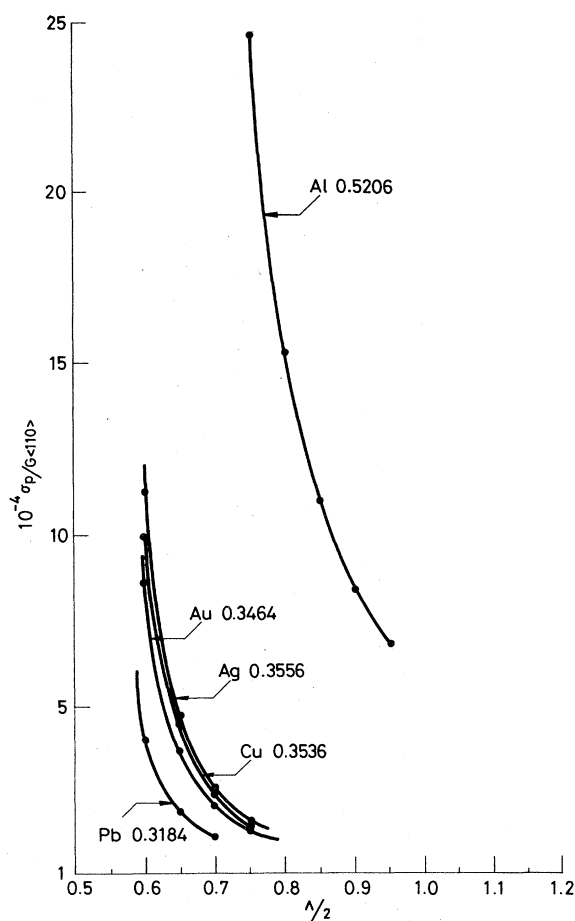

FIG. 6. Plot of Peierls stress as function of maximum strain parameter Λ for various fcc metals. Numbers listed are the P value for each metal as calculated in Table II. The surface energy can be obtained from Λ derived from experimental σ_p.

TABLE IV. Estimation of surface energy from the experimental activation energy of dislocation internal friction by the TFK dislocation model.

Material	Expt. activation energy (eV)	Corresponding[a] Peierls stress $(10^{-4}\,G_{\langle 110\rangle})$	Est. $\Lambda/2$ [b]	Est. surface[c] energy $(10^3\,\mathrm{erg/cm^2})$
Cu	0.122	5.03	0.640	1.497
Ag	0.124	6.22	0.630	1.077
Au	0.158	11.06	0.598	0.920
Al	0.250	23.49	0.748	1.299
Pb	0.058	5.16	0.588	0.387

[a] According to Seeger's double-kink–generation theory. See Ref. 15.
[b] Refer to Fig. 6.
[c] According to Eq. (11).

(1) The uncertainty of the accuracy of the surface energies, which were obtained in the high-temperature regime, whereas most of the internal-friction experiments were performed at low temperature.

(2) The inaccuracy of our TFK representation of a true edge dislocation. This might arise from the oversimplified nature of the Frenkel-Kontorova model itself, the force law used in the analysis as well as the assumption that the law around the ruptured dislocation center does not change from that of the perfect crystal.

(3) The question of the accuracy of Seeger's derivations in terms of continuum mechanics in the interpretation of the Bordoni relaxation peak. Since the kink energy can only be calculated accurately by atomistic model, elastic continuum theory is only an approximation.

Any one of these factors could cause an order-of-magnitude error in the calculated Peierls values. In spite of this, the results of our calculations are still within order-of-magnitude agreement. The more striking fact is that the corresponding variations between the experimental values and our calculated values for the metals examined are correlated. This provides more evidence for the excellency of the TFK model. More accurate predictions of the Peierls stresses, or the proof of the effectiveness of the model, depend on the availability of the accurate surface free energies at low temperature, which has long been difficult to obtain by experiment. However, if we use the experimental Peierls stresses given in the last column of Table II and reverse the analysis, we will be able to estimate the surface energies of these metals. This can only be performed graphically by using the curves shown in Fig. 6, where a stress value corresponds to a value of Λ; therefore the surface energy can be calculated, according to its definition. The results are listed in Table IV. It is interesting to see that the estimated surface energies are close to the values we used in Table I. This further confirms the effectiveness of our model. Incidentally, the analysis provides a method of estimation,
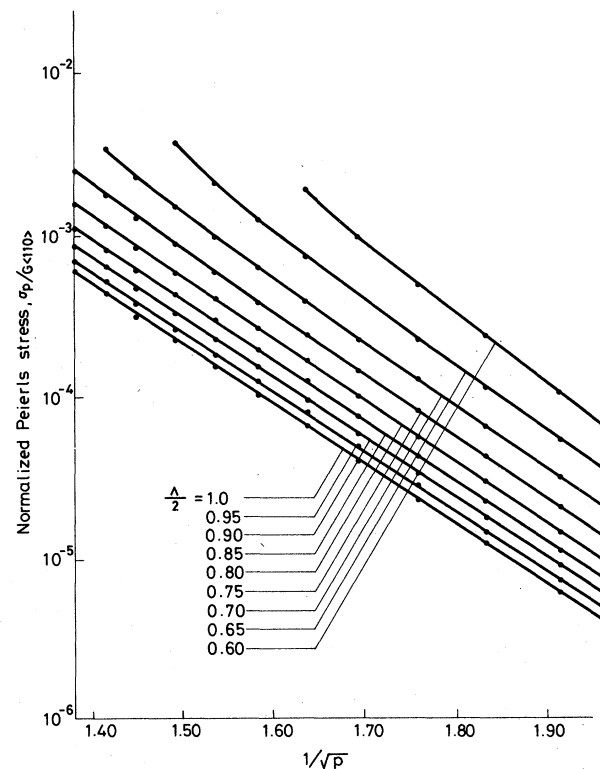

FIG. 7. Plot of Peierls stress as function of dislocation width parameter $P^{-1/2}$ defined in Hobart's analysis. Note that nearly straight lines in the plot for various Λ shows that the definition of dislocation width is still applicable to our nonlinear force model, except for high-stress regime where P is large and corresponding to narrow dislocation.

through the dislocation—internal-friction experiment, of the surface energy, or perhaps more directly, the interatomic force and the theoretical bond strength, f_0, of plastic materials. Therefore the problem of plasticity and the brittleness of a pure material can probably be overcome and directly compared from this point of view.

It is also astonishing that the simple sinusoidal force form can produce such a good agreement with experiment. However, if one views that any complicated force form can be expanded in terms of our sinusoidal force as the fundamental mode and its corresponding high harmonics, then the energy cancellation which results in a small Peierls barrier not only exists between the right-hand part and the left-hand part of the dislocation center for the fundamental mode, but also exists in the domains of each part itself for the high harmonic force components. This argument also applies to the harmonic substrate potential used in our model and is supported by Tyson's numerical calculation.[6]

The dislocation width, which is widely used in all models as a characteristic parameter, seems to be worth checking in our model, although a nonlinear force has been used in the analysis. This is shown in Fig. 7, where the logarithm of the Peierls stress is plotted as a function of the width parameter, $P^{-1/2}$. The nearly straight line obtained for various maximum strain parameter Λ indicates that the dislocation width as defined in Hobart's model[5] is still meaningful except in the regime of high Peierls stress of above 10^{-3} G.

V. CONCLUSIONS

The conventional Frenkel-Kontorova model has been modified into a tension-type Frenkel-Kontorova structure, which represents a more realistic edge-dislocation movement. The sinusoidal force law as the interatomic force with its parameters derived from the simple tension and the anisotropic conditions has been used and is logically explainable. Calculations of the Peierls stress by the TFK model have shown good agreement with Seeger's interpretation of data on several fcc crystals. The best fit is to the silver. It suggests that the Peierls hindering is largely caused by these tension atoms just below the slip plane. Incidently, the analysis also suggests a way of estimating the surface energy of solids from the dislocation—internal-friction experiment. Other potential laws and their relationships to other crystal properties, such as heat of sublimation, could also be used or evaluated by the analysis under appropriate formulations.

In principle, more accurate descriptions of an edge-dislocation migration can be achieved by extending the one-row dislocation to the two- or more-row models. Evidently, the adding of compressive rows will not strengthen the Peierls value directly, but it could help the relaxation of tension atoms and therefore lead to a more accurate result. Applications of the model to bcc materials and accounting for the temperature effect, therefore, to interpret more dislocation-related phenomena are also encouraging future extensions.

[1]R. E. Peierls, Proc. Phys. Soc. London 52, 23 (1940).

[2]F. R. N. Nabarro, Proc. Phys. Soc. London 59, 259 (1947).

[3]J. Frenkel and T. Kontorova, Phys. Z. Sowjetunion 13, 1 (1938).

[4]V. L. Indenbom, Sov. Phys. Cryst. 3, 193 (1958).

[5]R. H. Hobart, J. Appl. Phys. 36, 1944 (1965); 36, 1948 (1965).

[6]W. R. Tyson, in *Interatomic Potential and Simulation of Lattice Defects*, edited by P. C. Geblen, J. R. Beeler, Jr., and R. I. Jaffee (Plenum, New York, 1972).

[7]R. E. Reed-Hill, *Physical Metallurgy Principles*, 2nd ed. (Van Nostrand, New York, 1973), Chap. 20, pp. 847–850.

[8]H. Conrad, Acta Met. 6, 339 (1958).

[9]A. Maradudin, J. Phys. Chem. Solids 9, 1 (1959).

[10]R. Hobart, J. Appl. Phys. 37, 3573 (1966).

[11]R. Hobart, in *Dislocation Dynamics*, edited by A. R. Rosenfield *et al.* (McGraw-Hill, New York, 1968), pp. 161–173.

[12]D. Kuhlmann-Wilsdorf, Phys. Rev. 120, 773 (1960).

[13]J. H. Weiner and W. T. Sander, Phys. Rev. 134, A1007

(1964).

[14]Y. Y. Earmme and J. H. Weiner, J. Appl. Phys. 48, 3317 (1977).

[15]A. Seeger, H. Donth, and F. Pfaff, Discuss. Faraday Soc. 23, 19 (1957).

[16]P. G. Bordoni, J. Acoust. Soc. Am. 26, 495 (1954).

[17]J. P. Hirth and J. Lothe, *Theory of Dislocation* (McGraw-Hill, New York, 1968), Chap. 8.

[18]A. Seeger and P. Schiller, in *Physical Acoustics*, edited by W. P. Mason (Academic, New York, 1966), Vol. III.A, Chap. 8.

[19]I. Frenkel, Z. Phys. 37, 572 (1926).

[20]A. Kelly, *Strong Solids*, 2nd ed. (Clarendon, Oxford, 1973), Chap. 1, p. 10.

[21]D. H. Niblett, in *Physical Acoustics*, edited by W. P. Mason (Academic, New York, 1966), Vol. III.A, Chap. 3.

[22]E. Orowan, Rep. Prog. Phys. 12, 185 (1949).

[23]A. Bondi, Chem. Rev. 52, 421 (1953).

[24]B. E. Sundquist, Acta Metall. 12, 67 (1964).

[25]G. Ehrlich, in *Interatomic Potential and Simulation of Lattice Defects*, Ref. 6.