in yield should also have been observed in the Cu(110) crystal unless a competing process, tending to increase the yield, is operative and effectively cancels the decrease in yield due to the shortening of the focused collision sequence with temperature. In the case of the Cu(111) crystal this implies that the shortening of focused collision sequences is the predominant effect.

Two other interpretations regarding the effects of thermal vibration of lattice atoms should be mentioned. An oscillating atom in the lattice has a higher probability of being found at the end points of its travel than at the center. The effect of thermal oscillations thus is such that lower lying atoms, which were previously shielded from bombarding ions by surface atoms, become more and more exposed as the amplitude of vibration increases. The net result would be an increase in the probability of collision between an ion and a lattice atom and an increase in the sputtering yield.[7,9,17] This effect may not be small since according to Menzel-Kopp and Menzel,[18,19] amplitudes of vibration of surface atoms of Cu and Ag are roughly five times as great as for atoms in the interior of the metal.

The other effect attributable to increased lattice vibration is the decrease in effective binding energy of the surface atoms with increasing target temperature. Increased vibration is of course accompanied by an increased average energy of the surface atoms. Therefore, surface atoms need receive a proportionally smaller amount of energy in a collision to be ejected from the surface. This too would tend to increase the sputtering rate. The effect of binding energy on sputtering thresholds, for example, has been considered by Harrison and Magnuson.[20]

The effect of temperature on the channeling process[21,22] would be similar to the effect on focused collision sequences. That is, the increased vibration would result in a decrease of the distance an atom could travel in a channel of the crystal, resulting in a decrease in the sputtering yield.

The changes in yields reported here are generally quite small, in some cases not much larger than the maximum expected experimental uncertainty. However, the effect is a very real one and in view of the variant behavior of different crystal planes warrants further theoretical and experimental investigation.

[17] A. L. Southern, W. R. Willis, and M. T. Robinson, J. Appl. Phys. **34**, 153 (1963).

[18] Chr. Menzel-Kopp and E. Menzel, Z. Physik **142**, 245 (1955).

[19] Chr. Menzel-Kopp and E. Menzel, Z. Physik **144**, 538 (1956).

[20] D. E. Harrison and G. D. Magnuson, Phys. Rev. **122**, 1421 (1961).

[21] M. T. Robinson and O. S. Oen, Appl. Phys. Letters **2**, 30 (1963); O. S. Oen and M. T. Robinson, *ibid.* **2**, 83 (1963); M. T. Robinson, D. K. Holmes, and O. S. Oen, Bull. Am. Phys. Soc. **7**, 171 (1962); M. T. Robinson and O. S. Oen, *ibid.* **8**, 195 (1963).

[22] J. A. Davies, J. Friesen, and J. D. McIntyre, Can. J. Chem. **38**, 1526 (1960); J. A. Davies, J. D. McIntyre, R. L. Cushing, and M. Lounsbury, *ibid.* **38**, 1535 (1960); J. A. Davies and G. A. Sims, *ibid.* **39**, 601 (1961); J. A. Davies, J. D. McIntyre, and G. A. Sims, *ibid.* **40**, 1605 (1962); J. A. Davies, F. Brown, and M. McCargo, *ibid.* **41**, 829 (1963); F. Brown and J. A. Davies, *ibid.* **41**, 844 (1963).

PHYSICAL REVIEW VOLUME 138, NUMBER 3A 3 MAY 1965

Motion of a Frenkel–Kontorowa Dislocation in a One-Dimensional Crystal*

W. Atkinson and N. Cabrera
Department of Physics, University of Virginia, Charlottesville, Virginia

(Received 4 December 1964)

An analytic solution is given for the equations of a linearized Frenkel–Kontorowa one-dimensional dislocation. It is shown that the motion of the defect with velocity v excites lattice vibrations with k given by $\omega(k)=vk$, where $\omega(k)$ is the dispersion of the lattice waves. At high velocity there is only one k excited (in one dimension) appearing at the back of the defect, so that the frictional force is very small, one order of magnitude smaller than the Peierls force. At low velocities, however, there are many waves excited appearing both ahead and behind the moving defect, and the frictional force increases to the point of making steady-state nonthermally activated motion impossible.

1. INTRODUCTION

The motion of singularities in a lattice, whether foreign particles or imperfections of the lattice, remains as yet a rather mysterious subject.

First of all, there is the low-velocity motion, under a small applied force, which is described by assuming that the energy received by the singularity during an elementary jump is dissipated rapidly into the solid in the form of lattice waves. The motion has then to be thermally activated in so far as every elementary jump has to be independently excited. There is no question that this assumption appears to fit many of the experimental conditions; however, to our knowledge, no simple justification has been given for the fact that lattice waves are capable of rapidly dissipating the energy under these conditions.

Secondly, and more important to us, is the question

* Work supported by the U. S. Atomic Energy Commission, Contract No. AT-(40-1)-2488.

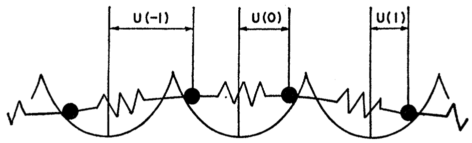

FIG. 1. The Frenkel–Kontorowa model of a dislocation. The potential illustrated is the one used in this paper.

of the possibility of a high velocity motion in which the singularity is allowed to acquire enough kinetic energy to be able to move through the lattice in a continuous fashion losing as much energy as it receives from a relatively small applied force. Such a possible motion was first considered years ago by Frank[1] in the case of a screw dislocation moving in a continuous elastic isotropic medium; he concluded that, provided the velocity was smaller than the sound velocity of shear waves, there was no mechanism for the dissipation of energy in the continuum so that the dislocation should be able to move at any velocity without the help of an external force. This is not correct, as pointed out by Leibfried[2] if we consider a hot solid, as the singularity will feel a resistance due to the scattering of the waves already excited in the solid. But even if a cold solid is considered, there should be an emission of sound waves due to the effective vibrations of the core of the dislocation as it moves through the lattice with periodicity a. Hart[3] estimated the frequency of these vibrations to be $\omega=4\pi v/a$, and the applied force necessary to compensate for the radiation loss to be very small and proportional to v^{-2}. This estimate implies therefore the possibility of a high velocity motion; however, the many simplifications introduced in it made it worthwhile to consider the problem again.

We will show in this and other papers that to discuss the radiation produced by a moving singularity, it is necessary to consider the discrete nature of the lattice itself. In general, the frequencies excited in the medium by a moving singularity are given by the relation $\omega(\mathbf{k})=\mathbf{v}\cdot\mathbf{k}$ where $\mathbf{k}$ is the wave vector of the lattice wave. Then, provided the dispersion relation $\omega(\mathbf{k})$ of the lattice and its periodicity in $\mathbf{k}$ are taken into account, it is easy to see that the high velocity continuous motion is possible because the range of possible excited wave vectors is small. This range increases rapidly for low velocities making energy dissipation very easy and a continuous motion impossible. In two or three dimensions there will never be a single frequency excited as was assumed by Hart.[3]

In this paper, we will discuss our problem on the simplest possible lattice model of a moving singularity, namely the classical Frenkel–Kontorowa[4] model of a one-dimensional dislocation. There is a substantial body of literature on this problem, particularly the papers by Frank and van der Merwe.[5] These authors, however, made a continuous approximation on the equations which resulted in eliminating the possibility of radiation being excited. Their conclusion therefore was that the singularity could move at any velocity, below the sound velocity, without the need of an applied force. Our treatment will solve the problem analytically without making any continuous approximation and will bring out both the necessity of radiation as well as its magnitude and its frequency spectrum.

In a recent paper, published while this paper was in preparation, Weiner[6] gives an approximate treatment of the motion of a Frenkel–Kontorowa dislocation, using a slightly more complicated potential than the one used in the present paper. He finds, as we do, that fast dislocation motion is possible at a stress considerably below that required to initiate motion. His treatment neglects the existence of radiative (nonlocal) modes and determines the energy loss as a result of an imperfect transfer of energy forward between successive local modes. This treatment appears to give reasonable answers, when the dislocation moves fast and there is only one radiative mode; it cannot, however, correctly describe the low velocity motion when many radiative modes are excited. Attention should also be called to a previous paper by Weiner and Sanders[7] which considers in particular the low velocity, thermally activated motion of the Frenkel–Kontorowa dislocation. This is clearly the only possible (classical) motion of this model at low velocities.

The type of treatment followed in this paper can be extended to the more general problem of the motion of singularities in three-dimensional lattices; this will be dealt with in a subsequent paper.

2. DESCRIPTION OF THE MODEL

The model illustrated in Fig. 1, consists of a line of atoms, mass m, with harmonic nearest-neighbor interactions of spring constant $m\omega_1^2$. The atoms are subject to a periodic potential, with the period equal to the equilibrium distance between neighboring atoms a. The model may be visualized as a chain of balls connected by springs resting on a washboard. A potential valley containing two (or no) atoms instead of one constitutes a defect. The displacement of the nth atom from the equilibrium position in the nth valley at the time t, is $u(n,t)$. Using the finite difference operator and its adjoint

$$\Delta_a f(x)=f(x+a)-f(x)\,,\quad \Delta_a{}^\dagger f(x)=f(x-a)-f(x)\,,$$

as a convenient notation, the potential energy may be

[1] F. C. Frank, Proc. Phys. Soc. (London) **A62**, 131 (1949).
[2] G. Leibfried and H. D. Dietze, Z. Physik **126**, 790 (1949).
[3] E. W. Hart, Phys. Rev. **98**, 1775 (1955).
[4] J. Frenkel and T. Kontorowa, Phys. Z. Sowjetunion **13**, 1 (1938); republished J. Phys. USSR **1**, 137 (1939).
[5] F. C. Frank and J. H. van der Merwe, Proc. Roy. Soc. (London) **A198**, 205 (1949); **A198**, 216 (1949); **A200**, 125 (1949); **A201**, 261 (1950).
[6] J. H. Weiner, Phys. Rev. **136**, A863 (1964).
[7] J. H. Weiner and W. T. Sanders, Phys. Rev. **134**, A1007 (1964).

written as

$$V=\sum_n \{\tfrac{1}{2}m\omega_1^2[\Delta_1 u]^2+U(u)\},$$

where $U(u)=U(u+a)$ is the periodic potential. To make the problem pseudolinear, we consider a potential which is piecewise parabolic, instead of the usual sine,

$$U(u)=\tfrac{1}{2}m\omega_0^2u^2, \quad |u|<\tfrac{1}{2}a.$$

We also introduce an external force σ, independent of position, which acts on each atom. This is equivalent to tipping the washboard and allows steady state motion of the defect. It acts on our defect in a manner similar to that of a shear stress on a dislocation in a crystal. The equation of motion is then

$$\begin{aligned} m[\ddot{u}+\omega_1^2\Delta_1^\dagger\Delta_1 u+\omega_0^2 u]&=\sigma, & -\tfrac{1}{2}a<u<\tfrac{1}{2}a,\\ &=\sigma+m\omega_0^2 a, & \tfrac{1}{2}a<u<3a/2.\end{aligned}$$

The continuous approximation mentioned in the introduction replaces the second difference in the previous equation by a second derivative.

3. STEADY-STATE MOTION

Steady-state motion of one defect with velocity v clearly means that if the $n=0$ atom moves from the 0th valley to the 1st valley, passing the discontinuity at $u=a/2$ at $t=0$, then the nth atom moves to the $(n+1)$th valley at $t=an/v$. The equation of motion is then

$$m[\ddot{u}+\omega_1^2\Delta_1^\dagger\Delta_1 u+\omega_0^2 u]=\sigma+am\omega_0^2 S(t-an/v),$$

where

$$S(x)=1 \quad x>0, \qquad S(x)=0 \quad x<0,$$

and $u(n)=a/2$ at $t=an/v$. We should emphasize that we are assuming the amplitude u of every atom to be small enough that at no time is there more than one defect in the entire chain. The solution of the previous equation depends on n and t only through the variable $x=an-vt$, which means that the displacement is stationary from the point of view of an observer moving with the defect. In terms of x the equation of motion can be written as

$$mL(x)u(x)=\sigma+am\omega_0^2 S(-x),$$

where

$$L(x)=v^2(d/dx)^2+\omega_1^2\Delta_a^\dagger\Delta_a+\omega_0^2,$$

and

$$u(0)=\tfrac{1}{2}a.$$

The solution of this equation may be found by Fourier analysis. Indeed, we write

$$L(x)e^{ikx}=L(k)e^{ikx},$$

where

$$L(k)=\omega^2-v^2k^2,$$

and $\omega(k)$ is the usual dispersion relation in the perfect lattice,

$$\omega^2=\omega_0^2+4\omega_1^2\sin^2\tfrac{1}{2}ka. \qquad (1)$$

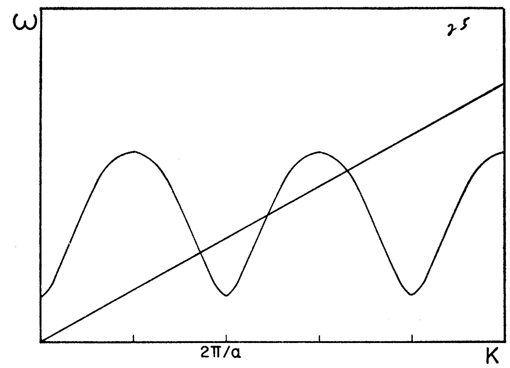

FIG. 2. Dispersion plot for sound waves in the Frenkel–Kontorowa model. Frequency ω as a function of wave number k. The radiative modes, solutions of $\omega=vk$, are given by the intersections between $\omega(k)$ and the straight line.

Using the representation of a step function, we obtain as a solution

$$u(x)=\frac{\sigma}{m\omega_0^2}-\frac{a\omega_0^2}{2\pi i}\int_{-\infty}^{\infty}\frac{e^{ikx}dk}{kL(k)}, \qquad (2)$$

provided only that the contour passes above the pole at the origin of the complex k plane. It should be mentioned that Eq. (2) can be rigorously justified, following Titchmarsh.[8] This solution is completely specified once the contour is entirely determined. The choice of contour is dictated by physical considerations. It must lie close to the real axis, so that the solution will not diverge for large x. The zeros of $L(k)$ determine of course the nature of the solution. There are two kinds of zeros: (a) A finite number of real zeros, which will be discussed in the next section and which represent the wave numbers of the acoustic radiation emitted by the defect. (b) An infinite number of complex zeros, which correspond to exponentially damped localized modes, which have zero amplitude at large distance from the defect and which describe the structure of the crystal around the defect.

The integral (2) can easily be evaluated by the method of residues, so that the solution comes out as a superposition of real waves and localized waves on one side of the defect and another similar superposition on the other side of the defect. This was to be expected on purely physical grounds. The Fourier analysis allows us to match the two superpositions around the defect in an elegant way.

4. THE CHARACTER OF THE ACOUSTIC RADIATION

A plane wave $\exp\{i(-\omega t+kan)\}$ with real k moving in the undisturbed crystal has a frequency given by (1) and if this is to be a part of our solution, of the form $\exp(ikx)$, we must have

$$\omega(k)=vk, \qquad (3)$$

[8] E. C. Titchmarsh, *Introduction to the Theory of Fourier Integrals* (Oxford University Press, New York, 1937).

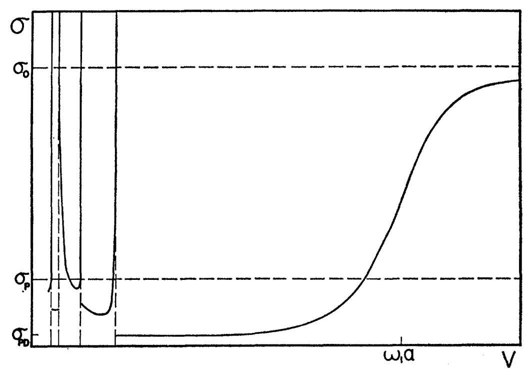

FIG. 3. Force σ on a moving dislocation as a function of velocity v. σ_P, the Peierls force, is the force required to initiate motion; $\omega_1 a$ the velocity of low frequency sound waves in the limit $\omega_0 \to 0$.

and therefore $L(k)=0$. The phase velocity of the excited radiation must be equal to the velocity of the defect. Equation (3) is illustrated in Fig. 2. The curve is $\omega(k)$, and the straight line has a slope v. At low velocity many modes are excited; at high velocity only one.

To determine the contour of integration, we impose a condition on the radiation emitted by the moving defect. All radiative modes with group velocity v_g greater than the defect velocity v must appear *only* ahead of the defect, all those with v_g smaller than v *only* behind. Noting that

$$v_g=\frac{d\omega}{dk}=v+\frac{1}{2v}\frac{1}{k}\frac{dL}{dk},$$

the contour must pass below (above) a zero of $L(k)$ when $kL'(k)$ is positive (negative). This determines completely our solution.

For certain critical velocities, the straight line in Fig. 2 becomes tangent to the curve $\omega(k)$. Two distinct modes of radiation merge. As the slope of the curve $\omega(k)$ is the group velocity, we see that the group velocity is equal to the defect velocity at tangency. The amplitudes of the corresponding modes diverge and our solution blows up.

5. RESISTANCE TO MOTION

The equation $u(0)=\frac{1}{2}a$ has not been used to determine the solution. Instead, it is used to determine the driving force σ. $u(0)$ is calculated from the series of residues and the value for σ is

$$\sigma=ma\omega_0^2\sum(1/k|L'(k)|), \tag{4}$$

where the sum extends over all real positive roots of $L(k)$. Thus the driving force is related to the radiation alone. Note that the choice of contour makes σ positive.

It is easy to show that formula (4) for σ could equally be derived from the conservation of energy; i.e., the work done on the crystal by the external force σ appears as radiation at the two sides of the defect.

A plot of σ as a function of v is given in Fig. 3, for the particular value $\omega_0/\omega_1=\frac{1}{2}$. The force σ is asymptotic to $\sigma_0=\frac{1}{2}m\omega_0^2a$, the applied force required to make the perfect chain move as a whole. On the same figure, we indicate the value of the Peierls force

$$\sigma_P=\sigma_0\omega_0/[(\omega_0^2+4\omega_1^2)]^{1/2}$$

in our model, namely the force required to start the defect moving. We notice first that $v=\omega_1 a$, which corresponds to the sound velocity, does not show any critical behavior as it would if $\omega_0\to 0$. On the other hand, there are singularities at all the resonances in amplitude every time the group velocity and the phase velocity coincide. This occurs more frequently at low velocities. Note that large amplitudes will violate our original assumptions about which atom is in which valley at what time. Thus the solution is not valid near a resonance, or for v larger than about $\omega_1 a$. This leaves one region of physical interest, roughly $\frac{1}{3}<v/\omega_1 a<1$, for the case $\omega_0<\omega_1$. In this range there is only one radiative mode which appears behind the defect. The possibility of motion at a lower velocity has not been carefully considered, but if allowed mathematically, it would likely not be physically interesting, as such motion would probably have $\sigma>\sigma_P$.

The minimum σ_{PD} indicated in Fig. 3, called by Weiner[6] the dynamic Peierls force, is the force required to sustain motion. It lies well below the force σ_P required to initiate motion: roughly $\sigma_{PD}/\sigma_0\approx(\sigma_P/\sigma_0)^2$.

The resonance phenomena depend entirely on the periodic dependence of frequency on wave number, and hence on the discrete character of the lattice. A continuous approach is clearly inadequate to describe the nature of the radiation. In the continuous approximation, which appears reasonable as $\omega_0/\omega_1\to 0$, no radiation is emitted; the defect is free to move at constant velocity with no driving force. Hobart's[9] more subtle approach considers a defect in a discrete lattice and radiation in a continuum. The results are fundamentally incorrect: the continuous model leads to the wrong frequencies as we have already indicated in the introduction.

It remains to comment on the significance of the singularities for $v_g=v$. We believe that these infinities are connected with the pseudolinear potential assumed in this paper as well as with the one dimensionality of the problem. This will be examined subsequently.

[9] R. Hobart, U. S. Air Force Office of Scientific Research AFOSR-647, 1961 (unpublished).