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Phonons radiated by moving dislocations in disordered alloys

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Résumé. — Nous utilisons la dynamique de réseau et les fonctions de Green de phonons pour systèmes désordonnés pour décire le spectre de phonons irradiés par une dislocation en mouvement dans un alliage désordonné. Nous évaluons l'atténuation de ces ondes par dispersion sur les impuretés et par excitation des modes localisés. Nous prédisons de larges amplitudes de vibration de ces impuretés et nous suggérons une modification du comportement diffusif autour des dislocations.

Abstract. — Lattice dynamics calculations together with the Green's function techniques for disordered systems are used to describe the phonon spectrum radiated by a moving dislocation in a random alloy. The attenuation of these waves by scattering at the impurities and by excitation of local modes is evaluated. Large amplitude vibrations of the impurities are predicted and modification of the diffusion behaviour in the neighbourhood of the dislocation is suggested.

1. Introduction.

The interaction of dislocation and impurities, or solute atoms in dilute alloys, plays an important role in several problems controlling the mechanical properties of crystalline materials. As examples we mention the solution hardening and softening, anelasticity, segregation [1] etc.

Most of the models of dislocations obtain forces from the derivatives of the interaction energies i.e. the energy difference between dislocation plus impurity in a given configuration and dislocation in a perfect lattice. This is essentially a static calculation.

In this work we investigate how lattice dynamics could take part in the complicated phenomena occurring in real materials. More precisely the question is to which extent lattice dynamics influences several well known effects such as the formation of Cottrell clouds, dislocation pinning or pipe diffusion. The aim of this work is to see whether the local modes introduced in the lattice by the presence of impurities can be resonantly excited to give rise to large amplitude localized vibrations. Depending on the symmetry of the associated eigenvectors, these large amplitude vibrations could strongly perturb the diffusion behaviour of these point defects.

2. The model.

2.1 Pure Crystal. — Dislocation dynamics in simple lattice models has been developed by Celli et al. [2] and Ishioka [3] based on the time-dependent Kanzaki force method [4]: A screw dislocation is introduced by external forces into an otherwise perfect simple cubic nearest-neighbour harmonic lattice at zero temperature. The time-dependent Kanzaki force is chosen so as to produce the uniform motion of an infinite straight dislocation. The uniform motion of a dislocation in a random substitute isotopic binary alloy has been treated by Caro et al. [Ref. [5], hereafter referred to as Paper I.]

The essential equation of the Green function formalism is the following:

\[ u_z^*(t) = \frac{1}{(2 \pi N)^{1/2}} \times \int_{-\infty}^{\infty} d\omega \sum_k e^{i(kr - \omega t)} G_{zz}(k, \omega) K_z(k, \omega) \]  

where \( u_z^*(t) \) is the z-component of the displacement.

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of an atom at position \( r \) and time \( t \); \( N \) is the number of atoms in the super-cell with periodic boundary conditions; the sum is over \( k \) in the first Brillouin zone. \( G_{zz}(\mathbf{k}, \sigma_3, \omega) \) is the diagonal element of the phonon Green function

\[
G_{zz}(\mathbf{k}, \sigma_3, \omega) = \frac{1}{M} \frac{1}{\omega^2(\mathbf{k}, \sigma_3) - \omega^2 - i \Gamma \omega}
\]

with

\[
\omega^2(\mathbf{k}, \sigma_3) = \frac{1}{M} \left( 4 \gamma_T \sin^2 \frac{k_x b}{2} + 4 \gamma_T \sin^2 \frac{k_y b}{2} + 4 \gamma_L \sin^2 \frac{k_z b}{2} \right)
\]

and the Kanzaki force, \( K_z(\mathbf{k}, \omega) \), is [4]:

\[
K_z(\mathbf{k}, \omega) = \left( \frac{N_x N_y}{N_z} \right) \frac{2}{\pi} \gamma_T b \delta_{k_r,0} \times \sin \frac{k_x b}{2} \frac{1}{\omega - i \epsilon} \sum \delta_{k_y} + G_y, \omega/v.
\]

In these expressions \( M \) is the mass of the atoms, \( \omega^2(\mathbf{k}, \sigma_3) \) is the dispersion relation for phonons with \( z \)-polarization, \( \Gamma \) is the phonon damping and \( \epsilon \) is a small positive constant; \( \gamma_L \) and \( \gamma_T \) are the longitudinal and transverse force constants, \( b \) is the Burgers vector and also the lattice parameter and \( G_y \) is a reciprocal lattice vector \( G_y = \frac{2 \pi}{b} n, n = 0, \pm 1, \ldots \).

For details of the derivation of these expressions and numerical evaluation of equation (1) the reader is referred to paper I.

Coordinates and geometry of the screw axes are shown in figure 1. A plot of displacements of an atom immediately above or below the glide plane \( (x = 0) \), as a function of \( (r_y - vt) \) where \( v \) is the dislocation velocity, \( v = (0, v, 0) \), is shown in figure 2. Coordinates of atoms are denoted by \( r_i (i = x, y, z) \).

Two main components of the displacement are easily detected: one is the underlying step function producing a net displacement of \( b/2 \) on each atom from \( t = -\infty \) to \( t = +\infty \). The other is an oscillation with a main Fourier component, decaying with time or distance. The Fourier components of the displacements can be analytically calculated from equation (1). The result is:

\[
u_x(\omega) = \frac{b}{2^{1/2}} \frac{e^{-i \omega r}}{\pi^{3/2} \omega - i \epsilon} \int_{-\pi/b}^{\pi/b} dk_x \times \frac{e^{ik_x r} \sin k_x b/2}{4 \sin^2 \frac{\omega b}{2} v - i \frac{\Gamma \omega M}{\gamma_T} + 2(1 - \cos k_x b)}.
\]

The limit \( \Gamma \to 0^+ \) must be taken for the perfect lattice case whereas in the disordered alloys \( i \Gamma \omega M \) must be replaced by a complex self-energy \( \Sigma(\omega) \) corresponding to a configurational averaged Green function.
With the substitution $e^{i k_x b} = Y$, equation (2) reads

$$u^*_{k_x} (\omega) = \frac{b}{(2 \pi)^{3/2}} e^{-\frac{i \omega v}{v'}} \int \frac{Y^{S+1} - Y^S}{Y^2 - 2 Y \left( \sin \frac{\omega b}{2 v} - \frac{\omega^2 M}{2 \gamma_T} - \frac{i \Gamma \omega M}{2 \gamma_T} + 1 \right) + 1} \, \text{d}y$$

where $S = r_x / b$ and the integral is over the unit circle in the complex plane.

Let $Y_+$ and $Y_-$ be the two roots of the denominator of equation (3) and suppose $Y_+ \neq Y_-$. Noting that $Y_+ = 1$, we identify $Y_-$ such that $|Y_-| > 1$ and $|Y_-| < 1$. In fact $|Y_-| = |Y_+|$ might only occur for $\Gamma = 0$. Only $Y_-$ falls inside the unit circle, therefore equation (3) can be easily integrated to give:

$$u^*_{k_x} (\omega) = \frac{b}{(2 \pi)^{1/2}} \frac{Y^S_+ - Y^S_-}{(\omega - i \epsilon)(Y^S_+ - Y^S_-)}.$$

Figure 3 shows $|u_{k_x} (\omega)|$, equation (4), for $S = 1$, $M = 1$, $\gamma_T = 1$, $b = 1$, $\Gamma = 10^{-3}$ and two values of dislocation velocities $v = 0.1 c$ and $v = c$, with $c$ the transverse sound velocity $c = b (\gamma_T / M)^{1/2}$.

Several peaks compose the Fourier spectrum of displacements shown in figure 2, superimposed to a $1/\omega$ dependence, which is the Fourier transform of the step function. Almost all peaks disappear for velocities near the sound velocity, but one, at $\omega_0^2$, around 0.66 of the maximum frequency $\omega_{max}^2 = 4(2 \gamma_T + \gamma_L)/M$. (The appearance of $\gamma_L$ here is only to give a proper definition of the maximum frequency of the perfect lattice. In the model we are dealing with only $\gamma_T$ is relevant).

The appearance of such peaks is related to the simultaneous existence of zeros in the real part of the denominator of equation (2) and in its derivative with respect to $k_x$. These peaks become non-integratable divergences in the limit $\Gamma \rightarrow 0^+$ if also $\partial \omega (k_x, k_y) / \partial k_x = v$. For our choice of dislocation velocities this singularity does not appear.

Null derivatives with respect to $k_x$ appear at $k_x = 0$ or $k_x = \pm \pi / b$ where $2 \gamma_T (1 - \cos k_x b)$ equals 0 or $4 \gamma_T$. Consequently the peaks appear at $\omega$ satisfying

$$f(\omega) = 4 \sin^2 \frac{\omega b}{2 v} - \frac{M}{\gamma_T} \frac{\omega^2}{\gamma_T} = \left\{ \begin{array}{ll} 0 & \text{for } \omega < 4 \\ -4 & \text{for } \omega > 4 \end{array} \right.$$

For velocities lower than the sound velocity, $c$, the function crosses the $\omega$-axis and the $y = -4$ axis several times giving rise to several peaks in the spectrum as shown in figure 3. For $v = c$ the function crosses the $y = -4$ axis only once giving a single peak in the spectrum.

In conclusion at least one peak appears at any dislocation velocity. Their amplitude is not lowered by lowering the dislocation velocity, which is a consequence of the snapping bond model used to describe the interatomic forces [2]. In fact even in the cases of a quasistatic macroscopic motion, microscopically the motion is decomposed into a very slow climbing of the Peierls hill and a fast falling down to the Peierls valley. This second part of the motion produces the large amplitude and high frequency peaks on the spectrum.

The preceding analysis gave nothing else but the same selection rules for phonon excitation in this particular model of dislocation dynamics already discussed by Ishioka [3] in one dimension and Celli et al. [2] in two dimensions. It is to note that for these frequencies the group velocity in the $x$ direction, $\partial \omega / \partial k_x$, is zero so that waves do not carry energy perpendicularly to the glide plane.

Although the peak heights depend on the phonon damping at those particular frequencies, we restrict ourselves to analyse the one corresponding to the highest frequency, $\omega_m$ (i.e. the one corresponding to $f(\omega_m) = -4$) which appears to be always the highest. In order to get analytic results on how the peak height decreases with the distance perpendicular to the glide plane let us approximate the two roots of the denominator in equation (2) to order $(\Gamma)^{1/2}$

$$y \approx -1 \pm \left( \frac{\Gamma \omega_m}{2} \right)^{1/2} \pm i \left( \frac{\Gamma \omega_m}{2} \right)^{1/2}.$$
then equation (4) becomes
\[ |u^S_m|^2 = \left( 1 - \frac{\Gamma \omega_m}{2} \right) S = e^{\frac{S^2}{2} \ln \left( 1 - \frac{\Gamma \omega_m}{2} \right)} \] (6)
i.e. it is an excitation exponentially localized around the glide plane. In the perfect harmonic crystal, \( \Gamma = 0 \), it propagates away without attenuation. At high concentrations of impurities this approximation fails because the imaginary part of the self-energy is no longer small. This is discussed in the next section.

2.2 Crystal with Low Concentrations of Solute Atoms. — The analysis of the lattice dynamics in the presence of impurities or solute atoms must be done in two different ways. On one hand how the amplitude of these particular waves decreases when propagating through the crystal. Part of their energy is transferred to other extended modes by scattering, or is lost by excitation of local modes around the impurities. To study this damping it is necessary to know the response function of the crystal containing a random distribution of impurities. In this way the attenuation could be obtained as a function of distance from the dislocation, concentration and impurity parameters.

On the other hand, a local description of an isolated impurity is necessary in order to know how local modes could be excited. The excitation of local modes would be produced by phonons whose frequencies are determined by the peaks in the Fourier spectrum (Fig. 3). These propagating waves are evidently inside the phonon band. Impurity modes which could resonantly absorb this energy are thus in-band or resonant modes whose eigenvectors are characterized by a concentration of displacements in the neighbourhood of the impurity. As a consequence of this absorption of energy, the amplitude of the impurity motion could rise up to levels significantly higher than those of its neighbours. This is a very peculiar situation of selective excitation which could affect the dynamics of diffusion near the core of dislocations. In fact if the eigenmode coincides with a reaction coordinate for diffusion, the impurity atom would need much less thermal energy to overcome the saddle point configuration.

It is out of the scope of this paper to calculate this enhanced diffusion effect quantitatively. It would be of small interest to perform calculations in such a simple model of harmonic, nearest neighbours, simple cubic crystal. This model allows us just to see this new effect of the lattice dynamics description of dislocation motion.

Let us proceed further on the analysis of the damping. A way to study the attenuation of a wave propagating in random media is through the configurational-averaged response function of these systems. We restrict ourselves to the simplest case of diagonal disorder (isotopic defect). The dislocation dynamics in this framework has been treated in paper I. In the present problem, equation (2) must be modified just by changing \( i \Gamma M \omega^2 \) for a complex self-energy \( \Sigma(\omega) \); the real part of \( \Sigma \) represents a shift of the eigenfrequencies and the imaginary part is inversely proportional to the phonon lifetime. The calculation of this self-energy in the Averaged-T-matrix-Approximation (ATA) [6] gives
\[ \Sigma(\omega) = \frac{\omega^2}{1 + G^{00}(\omega^2)} \]
where
\[
t(\omega) = + \frac{c_B (M_B - \langle M \rangle) \omega^2}{1 - (M_B - \langle M \rangle) \omega^2 G^{00}(\omega^2)} + \frac{(1 - c_B) (M_A - \langle M \rangle) \omega^2}{1 - (M_A - \langle M \rangle) \omega^2 G^{00}(\omega^2)}
\] (7)
where \( c_B \) is the concentration of atoms with mass \( M_B \), \( G^{00}(\omega^2) \) is the diagonal element of the Green function in the Virtual Crystal Approximation [7] and \( \langle M \rangle \) is the mean mass : \( \langle M \rangle = c_B M_B + (1 - c_B) M_A \). In what follows we consider the light isotope \( M_B = M_A/3 \).

Figure 4 shows the Fourier transforms of the atomic displacement for dislocation velocity equal to

![Figure 4](https://example.com/figure4.png)

Fig. 4. — Same as figure 3 for \( v = c \) and different concentration of B-atoms : a) \( c_B = 0 \); b) \( c_B = 0.25 \); c) \( c_B = 0.5 \); d) \( c_B = 0.75 \); e) \( c_B = 1 \).

the sound velocity at different concentrations of B-atoms. It is observed that the main peak position shifts towards higher frequencies as the concentration of B-atoms increases.

As in the perfect crystal case the attenuation of this wave, or more precisely the profile of the wave since its wave vector is \( k = \left( -\frac{\pi}{2b}, \frac{\omega}{v}, 0 \right) \), at posi-
tion \( r = (S, 0, 0) \) is approximately given by:

\[
|\mu_s^S(\omega_m)| = \left(1 - \frac{\Gamma'(\omega_m)}{2}\right)^{\frac{1}{2}} S \tag{8}
\]

but now \( \Gamma'(\omega_m) = \text{Im} \Sigma(\omega_m) \).

Although the ATA approximation gives zero damping for frequencies greater than the band edge of the virtual crystal, it is a good approximation because the frequencies we are interested in, associated with the peaks in the displacement spectrum, are always inside the virtual crystal band.

The damping of the highest peak as a function of concentration is shown in figure 5.

This figure shows that, for a fixed mass relation, the damping of a given peak, which is a measure of the spatial localization of the dislocation induced phonon radiation, depends on \( c_B \). Finally figure 6 shows \( \lambda = -\ln \left(1 - \left(\text{Im} \Sigma(\omega)\right)^2\right) \) the characteristic length of the approximated exponential decrement of amplitude, equation (6) and equation (8), as a function of concentration of B-atoms. It is observed that the existence of these peaks in the Fourier spectrum is restricted to the near-core of the dislocation in dilute alloys.

3. Discussion.

In this model of nearest neighbour interactions, \( x, y \) and \( z \) displacements are not coupled to each other, thus the radiated phonon spectrum has \( z \)-polarization or, in general, polarization along the Burgers vector of the dislocation. Consequently any effect on the diffusion behaviour of solute atoms due to the excitation of resonant modes should manifest itself as pipe diffusion — or parallel diffusion — in the case of screw dislocations, and as perpendicular diffusion in edge dislocations. Parallel or perpendicular refers to the dislocation line, not to the Burgers vector.

Although the frequencies corresponding to the peaks in the Fourier spectrum depend on the dislocation velocity, an oscillating dislocation loop, such as those measured in internal friction or ultrasonic attenuation experiments \[8\], will radiate at almost every frequency in the spectrum during a complete cycle. This seems to indicate that for almost any impurity there will be a fraction of the periodic motion where the energy radiated will be resonantly absorbed by the impurity. In this way quantitative details of the model become irrelevant and an assertion that this effect could be observable in real materials becomes plausible. These radiations are not related to those described in the non-linear continuum string model which are harmonics of the driving frequency.

Our result suggests that this anisotropic diffusion enhancement could affect the filling rate of the sinks represented by dislocation nodes. In fact an impurity atom attracted to the nodes by an elastic interaction would have an enhanced mobility parallel to the dislocation line near a screw dislocation. In the same way an oscillating edge dislocation would affect the impurity mobility in a plane perpendicular to the line. This effect, together with the elastic interaction would participate in defining the profile of the Cottrell atmosphere.

Present-day techniques applied to the study of dislocation motion, such as the coupled ultrasonic-low frequency measurements \[9\], seem to be sensitive enough to follow the kinetics of the Cottrell cloud and therefore to test the validity of our assertion. Experimental results in this field would be
of great importance to improve microscopic models of dislocations.

From the point of view of the relevance of the results obtained in the framework of the snapping-bond model, we would like to stress that the most important fact is that infrasonic dislocation motion is dissipative. This is not just a consequence of the simplicity of the model. The discrete nature of the lattice introduces dispersion. The dislocation, viewed as a superposition of external Kanzaki forces producing the desired topology, requires long wavelengths to be formed as well as wavelengths comparable to the lattice spacing. Therefore to maintain the wave packet undistorted, energy must be supplied.

In a recent paper [10] it has been formally shown that the equation of motion of a dislocation in an elastic continuum under external forces is a Newton equation with the Peach-Koehler terms plus a term proposed by Eshelby, provided that radiation reaction is not considered, i.e. as long as velocity is lower than sound velocity and acceleration is not too large.

The elastic continuum is a dispersionless medium where propagation of all transverse waves is described by a single transverse sound velocity c. In a lattice dispersion implies that each wave has its own group velocity \( v_g = \frac{\kappa_w(k)}{\omega} \) whose maximum value appears near \( k = 0 \) and equals the transverse sound velocity of the equivalent continuum medium. As a consequence, the dislocation running at any velocity always goes faster than some lattice waves and this implies dissipation. Therefore the continuum models of dislocations must have a viscous term as phenomenologically proposed long ago [11]. Although a formal derivation has only recently been made [12].

Another implication of our result is related to the question of how materials generate the density of dislocations required to accommodate arbitrary strains at high strain rates.

Recent molecular dynamics calculations on the 2-D Frenkel and Kontorova model show [13] a possible way of generation of dislocation loops in the wake of a moving dislocation. The authors interpreted this effect as due to the distortion caused by the emitted phonons and conclude that only when dislocations approach the speed of sound the amplitude of the radiated waves would be high enough to produce this effect. In our work it is shown that the amplitude of the emitted phonons is not simply related to the velocity in the high velocity region but a complicated consequence of selection rules for excitation which are model dependent but certainly existing for a real material.

By considering nearest neighbours and isotopic defects our model explicitly discards one of the most important interactions which is the elastic one. Only a full calculation with relaxation around defects could give an insight about the importance of the local mode excitation as a source of dislocation damping. The possibility of this source of dissipation was originally proposed by Takamura et al. in 1963 [14].

Finally it should be pointed out that a large number of interactions have already been extensively treated using different models [15, 16]. However, the question of what is the relative importance of each interaction mechanism remains without a conclusive answer.

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