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A lattice-dynamics model of the interaction of a dislocation with point defects

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Résumé. — Nous considérons un modèle de dynamique du réseau pour une dislocation vis, rectiligne, qui se déplace dans un réseau cubique simple avec des liaisons entre premiers voisins (modèle dit du « snapping bond »). L'effet sur le réseau, dû au mouvement de la dislocation, est décrit par une force-source dynamique, ou force de Kanzaki, et la réponse du réseau par la fonction de Green relative aux phonons. On introduit des défauts ponctuels isotopiques répartis de manière aléatoire. La fonction de Green du réseau avec défauts est calculée dans l'approximation de la matrice T moyenne (average T -matrix approximation). En égalisant l'énergie rayonnée par la dislocation en mouvement au travail fait par une contrainte extérieure, on obtient la relation entre contrainte appliquée et vitesse de la dislocation (en fonction de la concentration de défauts). Cette relation vitesse-contrainte montre que les défauts de masse, à travers leurs effets sur la dynamique du réseau, peuvent introduire un adoucissement dynamique en plus de l'effet bien connu de durcissement par solution solide.

Abstract. — We consider a lattice dynamics model of a straight screw dislocation moving in a simple cubic lattice with nearest-neighbour « snapping bonds ». The effect on the lattice of the dislocation motion is described by a dynamic source-force, or Kanzaki-force, and the lattice response by the phonon Green's function. A random array of isotopic substitutional point defects is introduced, and the average-t-matrix approximation of the configurational averaged Green's function is employed to describe the defect-lattice response. By using these quantities to calculate the energy radiated, as phonons, from the moving dislocation, and equating this energy to the work done by the applied stress, we obtain numerically the relation between the applied stress and dislocation velocity as a function of defect concentration. This stress-velocity relation shows that the site mass-change, through their global effect upon the lattice dynamics can introduce a dynamic lattice softening contribution to the usual solute hardening effect of the interaction between dislocation and point defects.

Introduction.

As a consequence of the great complexity of the plastic behaviour of metals and of the unanswered questions that this complex behaviour engenders, there is a continuing interest in microscopic models of dislocations. Among the unanswered question in this field there are those clearly involving microscopic interactions such as the interaction between a mobile dislocation and point defects, which suggest that we go beyond classical elastic continuum theory and investigate dislocations on a truly atomistic scale. Atomistic models of dislocation motion include one-

dimensional Frenkel-Kontorova models, computer simulation by molecular dynamics (with model potentials), and analytical solution based on the theory of lattice dynamics (with empirical force-constants). First principles theories at the electronic level, such as the works of Masuda and Sato [1-3], which yield the core structure, core energy, and Peierls stress of screw dislocations in bcc transition metals and dilute alloys, are based on procedures leading to static equilibrium and neglect all dynamical effects.

The idealized lattice-dynamical models of Celli and Flytzanis [4, 5] and of Ishioka [6] lead through diffe-

rent approaches to quantitative relations between the applied stress and dislocation velocity. The basic model of Celli and Flytzanis, for a screw dislocation moving in a simple cubic (SC), nearest-neighbour, harmonic lattice, with snapping bonds, was recast by Glass [7] in terms of a dynamic source-force (generalized from the Boyer-Hardy static force [8]) for arbitrary dislocation motion and of the phonon Green's function. One object of reference [7] was to derive expression amenable to straightforward generalization to take into account, for example, the dynamic effects of point defects, through a modified lattice response function. An expression for the energy dissipated by an harmonically oscillating dislocation in a perfect lattice was derived, and then the way in which point defects should change this expression was outlined.

In this paper, we follow up on the ideas of reference [7], by actually implementing the theory numerically, for the case in which the screw dislocation moves through the SC lattice containing a random array of isotopic mass defects. The effect of the defects is incorporated in the Green's function through use of the average- T -matrix (ATA) approximation. In order to deal with the added complication of the defects in a quantitative way, we simplify the dislocation motion to that of constant velocity. We calculate the relation between the applied stress and the dislocation velocity as a function of defect concentration, and we discuss the hardening (softening) of the crystal in light of the results.

Of course, such a model (in which thermal phonons and kinks do not exist) is strictly valid at $T = 0$ K. Nevertheless, for low temperatures, in which thermal creation of kink pairs [9] is unlikely, plastic deformation should occur only when the applied stress is high enough to push dislocations over the Peierls potential, and the mechanism envisaged here has relevance. One might thus compare our results for the effect of mass defects on the stress-velocity relation, to experimental measurements on solid solution hardening near $T = 0$ K.

The present model, which neglects force-constant changes due to the defects and lattice relaxation around the defects, does not include those well-known contributions to the interaction between dislocations and point defects that are calculated

in continuum theory, namely, the size misfit and modulus misfit contributions (reviewed in Refs. [10] and [11]). On the other hand, the effect of the altered masses, *via* the global change in the lattice dynamics, is totally absent from continuum theory. In fact, we find that the mass-change can add another term to the *dynamic* interaction between high-velocity dislocations and point defects.

The organization of the paper is as follows. First, we review some of the steps in reference [7] to obtain an expression for the power radiated as phonons from a moving screw dislocation, for the perfect lattice. This leads to an expression for the applied stress *versus* velocity, which is the same as the Celli-Flytzanis result [4], and which we have evaluated numerically for finite phonon damping (different from Ref. [4]). We then replace the perfect-lattice Green function with the ATA Green function and present the numerical solution of the stress-velocity relation as a function of defect concentration.

1. The model.

In the article by Glass [7] results are derived first for the arbitrary motion of a straight screw-dislocation, at position $\mathbf{R}(t)$, and then for the case of harmonic oscillatory motion, i.e., $\mathbf{R}(t) = \hat{y}bR_0 \cos \Omega t$, where bR_0 is the amplitude of vibration. Here we shall reproduce the most important steps of the calculation for the particular case of uniform motion (i.e. $\mathbf{R}(t) = \hat{y}vt$) in order to obtain the displacements and energy dissipation in the lattice containing one type of atom. The case of the isotopic substitutional alloy is treated in the next section.

Consider a simple cubic lattice in the harmonic approximation with nearest neighbour interactions. An infinitely long screw dislocation parallel to the Z -axis and intersecting the centre of a cube face is shown in figure 1. Following Boyer and Hardy [8], the Kanzaki force necessary to create the topology of the screw dislocation is given by :

$$K_i^m = \sum_{m,j} [\mathbf{r}^m, \mathbf{r}^n] \Phi_{i,j}^{m,n} b \delta_{i,z} \quad (1)$$

where m, n denote the atoms at $\mathbf{r}^m, \mathbf{r}^n$, i is the Cartesian direction, b is the Burger's vector (equal to the lattice parameter), Φ_{ij}^{mn} is the matrix of force constants and :

$$[\mathbf{r}^m, \mathbf{r}^n] = \begin{cases} + 1 (-1) & \text{if the } m\text{-}n \text{ bond crosses the cut-plane (but not through the dislocation line) and} \\ & \text{if } m \text{ is to the left (right) of } n. \\ + 1/2 (-1/2), & \text{if the } m\text{-}n \text{ bond crosses the dislocation line and } m \text{ is to the left (right)} \\ & \text{of } n. \\ 0 & \text{otherwise.} \end{cases}$$

The Kanzaki force, equation (1), in the co-ordinate system shown in figure 1, is :

$$K_i^m(t) = b \delta_{iz} \sum_{\mathbf{r}} [\theta(-r_x) \theta(r'_x) - \theta(r_x) \theta(-r'_x)] \times \theta(vt - r_y) \Phi_{iz}^{mn} \delta_{r_y, r'_y} \quad (2)$$

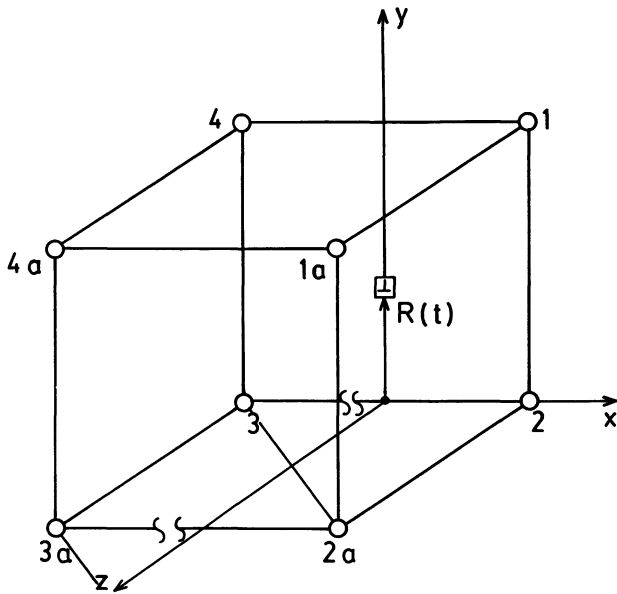


Fig. 1. — Geometry of the model considered : a simple cubic lattice containing an infinitely long screw dislocation along the Z-axis, moving in the y-direction, and intersecting the xy-plane at the position R(t).

where v is the dislocation velocity and $\theta(x)$ is the Heavyside function whose Fourier integral representation is

$$\theta(x) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} dk \frac{e^{ikx}}{k - i\epsilon}, \quad \epsilon \rightarrow 0^+.$$

It is useful to work in reciprocal space ; therefore equation (2) is Fourier transformed with respect to the discrete variables r_i ($i = x, y, z$) and the continuous variable t .

It is important to note that the condition of nearest neighbour-interactions appears through the matrix $\phi_{iz}^{rr'}$, reducing the sum over r_x to two terms. With the origin as shown in figure 1 [the position of the atom labelled (s, t, p) is $\mathbf{r} = (sb + b/2, tb, pb)$], the Fourier transform of equation (2) is $K_x(\mathbf{k}, \omega) = K_y(\mathbf{k}, \omega) = 0$ and :

$$K_z(k, \omega) = \frac{\sqrt{N_y N_z}}{\sqrt{N_x}} \frac{2}{\pi} \gamma_T b \delta_{k_z, 0} \sin\left(k_x \frac{b}{2}\right) \times \frac{1}{\omega - i\epsilon} \sum_{G_y} \delta_{k_y + G_y, \omega/v} \quad (3)$$

where γ_T is the transverse force constant, N_i ($i = x, y, z$) is the number of atoms in the direction i and G_y is a reciprocal lattice vector, $G_y = 2\pi n/b$, $n = 0, \pm 1, \dots$

As shown in paper I the displacements can be obtained from equation (3) and the phonon Green's functions for the perfect simple cubic lattice :

$$G_{ij}(\mathbf{k}, \omega) = \frac{1}{M} \delta_{ij} \frac{1}{\omega^2(\mathbf{k}, \sigma) - \omega^2 - i\Gamma\omega}. \quad (4)$$

In the particular model crystal under consideration G_{ij} is diagonal in i and j ; therefore the displacements produced by the Kanzaki force, equation (3), are only in the z -direction. Since there is no dependence of K_z^m on z , the relative displacement of atoms along the z axis is 0, implying that there are no waves propagating along the z axis. In conclusion, waves will propagate in the x - y plane with $\sigma_3 = (0, 0, 1)$ polarization. For those waves, the phonon dispersion relation entering equation (4) is :

$$\omega^2(\mathbf{k}, 3) = \frac{1}{M} \left\{ 4 \gamma_T \sin^2 \frac{k_x b}{2} + 4 \gamma_T \sin^2 \frac{k_y b}{2} + 4 \gamma_L \sin^2 \frac{k_z b}{2} \right\} \quad (5)$$

where γ_T and γ_L are the transverse and longitudinal force constants respectively. Finally, the displacements are :

$$u_z^r(t) = \frac{1}{\sqrt{N_x N_y N_z} \sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega \sum_{\mathbf{k}} e^{i(\mathbf{k}\cdot\mathbf{r} + \omega t)} K_z(\mathbf{k}, \omega) G_{zz}(\mathbf{k}, \omega)$$

which after some algebra becomes :

$$u_z^*(t) = \frac{b}{2\pi^2} \int_{-\pi}^{\pi} dK_x \int_{-\infty}^{\infty} dK_y \frac{\sin(K_x/2) \exp\left[i\left(\frac{r_y}{b} + \frac{vt}{b}\right)K_y\right] \exp\left(i\frac{r_x}{b}K_x\right)}{(K_y - i\varepsilon) \left[4\left(\sin^2\frac{K_x}{2} + \sin^2\frac{K_y}{2}\right) - \left(\frac{v}{c}\right)^2 K_y^2 - i\Gamma K_y\right]} \quad (6)$$

where c is the sound velocity.

As quoted in reference [7] this result is the same as obtained by Celli and Flitzanis starting from the Newtonian equation of motion (see Eq. (2.9) in Ref. [4]).

The energy radiated in the phonon field is equal to the work done by the Kanzaki force. The power dissipated into the whole crystal is :

$$\dot{W}(t) = \sum_{m,i} K_i^m(t) \cdot \frac{du_i^m(t)}{dt}. \quad (7)$$

From equation (6)

$$i\dot{u}_z^*(t) = \frac{iv}{2\pi^2} \int_{-\pi}^{\pi} dK_x \int_{-\infty}^{\infty} dK_y \sin\frac{K_x}{2} \frac{\exp\left[i\left(\frac{r_y}{b} + \frac{vt}{b}\right)K_y\right] \exp\left(i\frac{r_x}{b}K_x\right)}{\left[4\left(\sin^2\frac{K_x}{2} + \sin^2\frac{K_y}{2}\right) - \left(\frac{v}{c}\right)^2 K_y^2 - i\Gamma K_y\right]} \quad (8)$$

and from equation (3)

$$K_z^m(t) = \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{N_x N_y N_z}} \int_{-\infty}^{\infty} d\omega \sum_{\mathbf{k}} e^{i(\mathbf{k}\cdot\mathbf{r}^m + \omega t)} K_z(\mathbf{k}, \omega) \quad (9)$$

Using equations (8) and (9) in equation (7), we obtain :

$$\dot{W}(t) = -i4\pi N_z \gamma_T b v \int_{-\pi}^{\pi} dK_x \int_{-\infty}^{\infty} dK_y \frac{\sin^2 K_x/2}{\left(K_y - i\varepsilon \frac{b}{v}\right)} \times \frac{1}{4\left(\sin^2\frac{K_x}{2} + \sin^2\frac{K_y}{2}\right) - \left(\frac{v}{c}\right)^2 K_y^2 - i\Gamma K_y}. \quad (10)$$

In the limit $\varepsilon \rightarrow 0$ we can split the integrand in this formula into its real, R , and imaginary, I , parts as follows :

$$R = \sin^2\frac{K_x}{2} \left[P\left(\frac{1}{K_y}\right) \operatorname{Re} \left\{ G_{zz}\left(\mathbf{K}_{\perp}, \frac{v}{c} K_y\right) \right\} - \pi\delta(K_y) \operatorname{Im} G_{zz}\left(\mathbf{K}_{\perp}, \frac{v}{c} K_y\right) \right] \quad (11a)$$

$$I = \sin^2\frac{K_x}{2} \left[P\left(\frac{1}{K_y}\right) \operatorname{Im} G_{zz}\left(\mathbf{K}_{\perp}, \frac{v}{c} K_y\right) + \pi\delta(K_y) \operatorname{Re} G_{zz}\left(\mathbf{K}_{\perp}, \frac{v}{c} K_y\right) \right] \quad (11b)$$

where \mathbf{K}_{\perp} is $K_x \hat{x} + K_y \hat{y}$ and P denotes principal value.

The integral of the first term in (11a) is zero because of its parity while that of the second is zero because $\operatorname{Im} G_{zz}(\mathbf{K}, \omega)$ is zero for $K_y = 0$ (note that Eq. (4) is the retarded Green's function whose imaginary part is proportional to ω , or to K_y in Eq. (10)).

The second term in equation (11b), when integrated over K_y reduces to $\pi/4$ and therefore only the first term in (11b) must be evaluated, namely

$$\dot{W}(t) = 4\pi M N_z \gamma_T b v \int_{-\pi}^{\pi} dK_x P \int_{-\infty}^{\infty} dK_y \frac{\sin^2 K_x/2}{K_y} \operatorname{Im} G_{zz}\left(\mathbf{K}_{\perp}, \frac{v}{c} K_y\right). \quad (12)$$

Equation (12) can also be obtained from a generalization to a system of many degrees of freedom of the

well known relation between the power transferred to a system by an external force $F(t) = 1/\sqrt{2\pi} \int d\omega F(\omega) e^{i\omega t}$ and its response function $G(\omega)$

$$\dot{W} = \int d\omega \omega |F(\omega)|^2 \text{Im } G(\omega).$$

The function $\text{Im } G_{zz}\left(\mathbf{K}_\perp, \frac{v}{c} K_y\right)$ in equation (12) has large values only for those \mathbf{K} where $\omega(\mathbf{K}_\perp) = \frac{v}{c} K_y$. As discussed by Ishioka [6] in one dimension, and Celli *et al.* [4] in two dimensions, this represents a selection rule for the excitation of lattice waves. When the phase velocity, $\omega(\mathbf{k})/k_y$, and the group velocity, $\partial\omega(\mathbf{k})/\partial k_y$, in the y -direction, equal the dislocation velocity, v , the energy transferred to that particular mode cannot escape the dislocation core, leading to a divergence of the integral in equation (12) in the case of null damping ($\Gamma \rightarrow 0$).

In order to impose conservation of energy, we must equate the power dissipated by the moving dislocation to the power dissipated by an external shear stress. Forces $\mathbf{F} = (0, 0, \pm F)$ applied to the faces zy at $x = \pm N_x b/2$ produce the necessary shear stress $\sigma = F/b^2 N_z N_y$. The work done by these forces is composed of two terms : an elastic and a plastic contribution. The total plastic work done on each surface atom is $F_{\text{at}} \frac{b}{2} = \sigma b^2 \frac{b}{2}$. The number of atoms per unit time which are displaced by the moving dislocation is $2 N_z \frac{v}{b}$. Therefore the power dissipated becomes

$$\dot{W} = \sigma b^2 v N_z. \tag{13}$$

Equating equation (13) to (12) we obtain the desired relation between external stress σ and dislocation velocity v as :

$$\frac{\sigma b}{\gamma_T} = \frac{\sigma}{\mu} = 4 \pi M \int_{-\pi}^{\pi} dK_x P \int_{-\infty}^{\infty} dK_y \frac{\sin^2 K_x/2}{K_y} \text{Im } G_{zz}\left(\mathbf{K}_\perp, \frac{v}{c} K_y\right). \tag{14}$$

The Peierls stress, σ_p , is the stress required under quasi-static conditions (in the absence of thermal motion) to move the dislocation from one stable equilibrium position to an adjacent one. In this model σ_p is just the stress necessary to produce a relative displacement of two atoms across the slip plane equal to $b/2$. When an external stress is applied to the crystal, the atomic displacements are the sum of the elastic deformation, $\varepsilon = \sigma/\mu$, and the strain field of the static dislocation. When considering the core atoms across the slip plane, for instance $r_1 = (b/2, 0, 0)$ and $r_2 = (-b/2, 0, 0)$, the Peierls stress should satisfy that $r_1 - r_2$ as a function of σ_p be equal to $b/2$:

$$|u^{r_1} - u^{r_2}| = \frac{b}{2} = \frac{\sigma_p b^2}{\gamma_T} + |u^{r_1} - u^{r_2}|_D. \tag{15}$$

Where $|u^{r_1} - u^{r_2}|_D$ represent the dislocation-induced relative displacement, given by equation (6) for $v = 0$ and the first term in the right hand side is the elastic contribution.

The static configuration of the core is just that given by the elastic continuum theory, i.e. $u^{(xyz)} = \frac{b}{2\pi} \text{artg } y/x$.

The static relative displacement for two core atoms across the slip plane is $b/4$ and then the Peierls stress, σ_p , is given by $b/2 = \sigma_p b/\mu + b/4 \rightarrow \sigma_p = \mu/4$. For any pair of nearest neighbour atoms very far from the dislocation the relative displacement is

given by $|u - u'| = \frac{\sigma b}{\mu}$ and the limit of cohesion, σ_L , is given by $|u - u'| = \frac{b}{2} = \sigma_L \frac{b}{\mu} \rightarrow \sigma_L = \mu/2$.

Equation (14) has been evaluated numerically for a value of the phonon damping $\Gamma = 0.001 c/b$. Note that the integrand has even parity in both integration variables and is zero for $K_y = 0$ so that numerical integration has been made for positive values of K_x and K_y . Also $\text{Im } G_{zz}(\mathbf{K}, \omega)$ is zero for $\omega > \omega_{\text{max}}$; in this case it is zero for $K_y = \frac{8c}{v}$. Finally the relative errors in a Gauss subroutine were fixed the first variable (K_x) and 10^{-3} for the second. Calculations for velocities from $v = 0$ at step of $\Delta v = 0.001 c$ were made in order to obtain the plot shown in figure 2.

Many interesting features are shown in this figure. Three distinct regions appear : for high velocities ($v > 0.4 c$) the movement is well defined ($\partial v/\partial \sigma > 0$) and similar to that of the continuum theory (in an elastic continuum with dissipation the $v - \sigma$ relation is linear characteristic of a viscous damping). This high velocity region is equivalent to that obtained by Celli and Flytzanis [4].

At intermediate velocities, the velocity-stress curve has regions of instability ($\partial v/\partial \sigma < 0$) and shows near-singularities in the stress at certain velocities (e.g. $v/c = 0.3$). The precise nature of these points

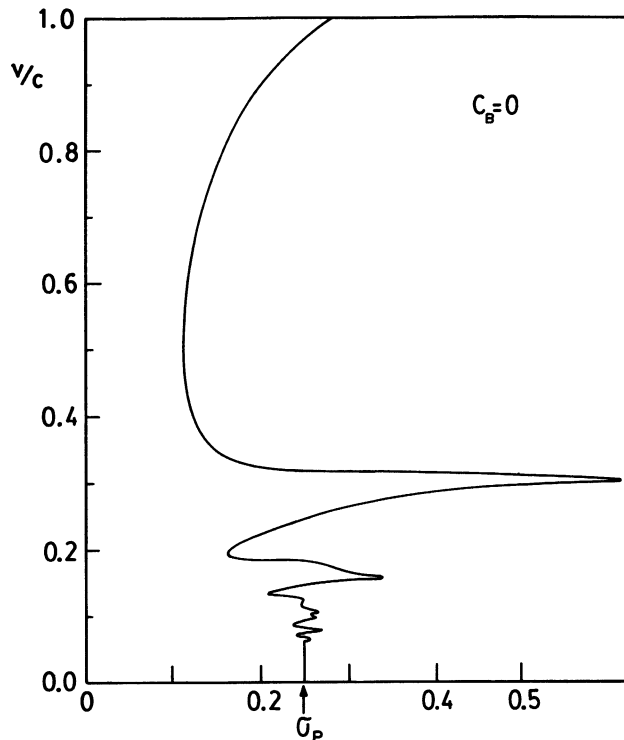


Fig. 2. — Dislocation velocity (divided by sound velocity), v/c , versus applied shear stress (divided by shear modulus), σ/μ , for a screw dislocation moving uniformly in a perfect cubic lattice.

of nearly divergent stress depends on the choice of the phonon damping parameter Γ , of which the value used here is an arbitrary one. In particular, when $\Gamma = 0$, there is a true singularity in the stress as discussed by Celli and Flytzanis [4]. In reference [4] these authors point out that these divergences occur at the critical velocities, at which a phonon propagates with the same phase and group velocity as the dislocation velocity. The energy radiated from the dislocation into such a lattice mode cannot escape from the dislocation core and thus the atomic vibrational amplitudes become large (infinite when $\Gamma = 0$), as does the stress necessary to maintain the motion. It is interesting to note that with an increase in the choice of Γ , the divergences found in reference [4] and the breakdown in the model that it represents, is here removed. In fact we shall see in the next section that when additional phonon damping due to the presence of point defects is introduced, the sharp spikes in the stress are even further reduced.

The region of low velocities, $v < 0.05 c$, is interesting since the results in this region may be compared to experiments: for example to measurements of the critical shear stress near 0 K (this being the minimum stress to start moving the dislocation from zero velocity). We notice that the limiting stress for $v \rightarrow 0$ in figure 2 equals the static Peierls stress evaluated in equation (15), in contrast to the results of Weiner [12] and Ishioka [6] in one dimensional models, where a

dynamic Peierls stress, lower than the static one, is found. Experiments on dislocation velocity under known stress pulses [13], near the critical stress, reveal dislocation velocities some order of magnitude lower than the sound velocity. At the lowest temperature reported in reference [13], 77 K, the dislocation velocity shows a rapid rise near the critical stress, as found here. Of course in the present simple model there are no other dislocations, defects or thermal phonons to slow down the dislocation, and there is no motion by dislocation bowing; our dislocation is always straight. The derivative $\partial v/\partial \sigma \rightarrow \infty$ for this $v \rightarrow 0$ region is characteristic of a sliding friction mechanism.

2. The influence of point defects.

The Green's function, equation (4), which enters the equation for the dissipation, equation (14), is the response function of the perfect crystal. Since it is just the imaginary part of this function that needs to be calculated, see (12), the dissipation of energy can be interpreted as a function of the local density of states or frequency spectrum $D(\omega^2)$:

$$D(\omega^2) = -\frac{M}{\pi} \text{Im} G_{zz}^{0,0}(\omega^2) \quad (16)$$

where

$$G_{zz}^{0,0}(\omega^2) = \frac{1}{\sqrt{N_x N_y N_z}} \sum_{\mathbf{k}} G_{zz}(\mathbf{k}, \omega).$$

The density of states for the simple cubic lattice is plotted in figure 3. It corresponds to the acoustic band which ends at $\omega_{\max}^2 = \frac{4}{M}(\gamma_L + 2\gamma_T)$.

The Green's function in equation (16) is defined through the Hamiltonian of the perfect lattice, H , as

$$G(E) = (H - E)^{-1}. \quad (17)$$

When impurities are present a perturbation term appears which in the site representation and for an isotopic substitutional impurity reads

$$V = \sum_{\mathbf{l}, \mathbf{l}'} (M_B - M_A) \Delta(\mathbf{l}) \frac{(\dot{u}_{\mathbf{l}}^i)^2}{2} = \sum_{\mathbf{l}} M_A \varepsilon(\mathbf{l}) \frac{(\dot{u}_{\mathbf{l}}^i)^2}{2} \quad (18)$$

where M_B is the mass of the impurity atom, M_A is that of the host atom, $\Delta(\mathbf{l})$ equals 1 if the site \mathbf{l} is occupied by an impurity atom and 0 otherwise and $\varepsilon(\mathbf{l}) = (M_B/M_A - 1) \Delta(\mathbf{l})$.

The formal solution for $G(E)$ is

$$G(E) = (H + V - E)^{-1} = \left(\frac{1}{P(E)} - V \right)^{-1} \quad (19)$$

where now $P(E) = (H - E)^{-1}$ is the perfect lattice Green's function. Equation (19) can be written as a Dyson equation

$$G(E) = P(E) + P(E) V G(E). \quad (20)$$

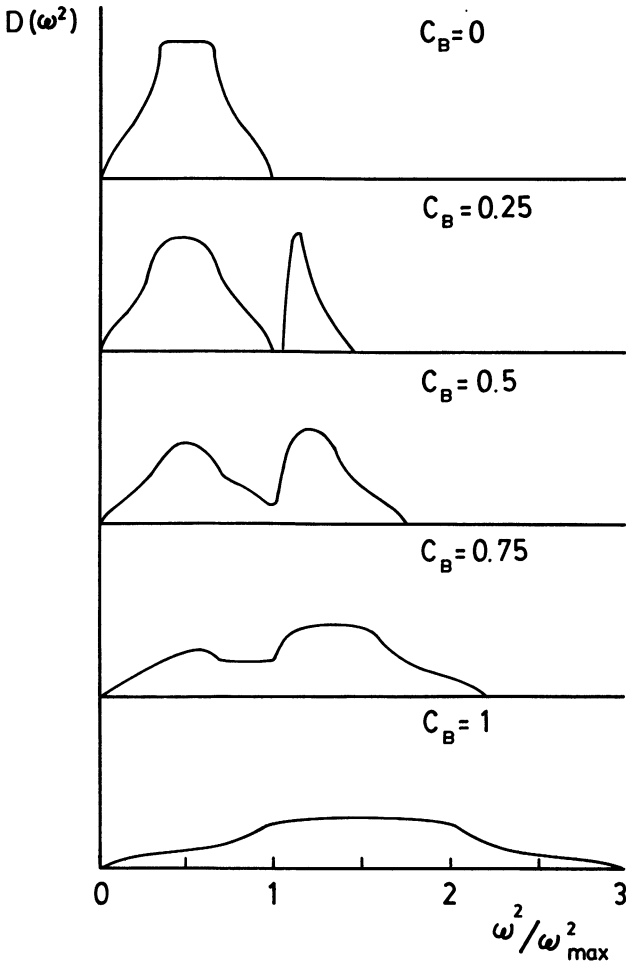


Fig. 3. — The phonon density of modes $D(\omega^2)$ for five different concentrations C_B of random mass-defects (mass M_B) in a simple cubic lattice (atomic mass $M_A = 3 M_B$), as used in the calculations for the dislocation motion.

Equation (20) is unsolvable because of the infinite dimension of the matrices and because the exact location of each impurity is unknown.

The problem of a dislocation moving in a crystal containing point defects should be solved for each

configuration of point defects and then the energy dissipated averaged over these configurations. The number of such configurations being infinite, one is forced to use a configurational averaged Green's function.

For an homogeneously random system the averaged Green's function has the translational symmetry of P and an equivalent Dyson equation can be written, like equation (20), in terms of a self energy [14] :

$$G(E) = P(E) + P(E) \Sigma(E) G(E). \quad (21)$$

Among the different approximations developed for $\Sigma(z)$, we shall adopt the T -matrix decoupling schema (see for instance Ref. [14]) where $\Sigma(E)$ is given by :

$$\Sigma(E) = C_B \frac{M_A \varepsilon \omega^2}{1 - (1 - C_B) M_A \varepsilon \omega^2 P(E)} \quad (22)$$

where C_B is the concentration of impurity B atoms in this way the averaged response functions becomes :

$$G(E) = (H + \Sigma(E) - E)^{-1}. \quad (23)$$

The density of states resulting from this approximation (i.e. $-M/\pi \text{Im } G_{zz}^{00}(\omega^2)$ with $G_{zz}^{00}(\omega^2)$ given by Eq. (23)) is represented in figure 3 for $M_B = M_A/3$ and several values of the concentration. For a low concentration of B-atoms a band of localized modes appear which enlarges with increasing concentration until the gap disappears. Reciprocally, starting from $C_A = 0$ the inclusion of heavy A atoms produces a peak of resonant modes in the low frequency region of the spectrum. The consequences of the self-energy term in equation (23) is that each mode at frequency ω is shifted by a quantity $\text{Re } \Sigma(\omega)$ and broadened by a quantity $\text{Im } \Sigma(\omega)$. (Note that in a random alloy, plane waves are no longer eigenstates.)

For $C_B = 1$ the effect of the self-energy term is just to change M_A into M_B and therefore the results is exact. The only differences between pure crystals A and B are the speeds of sound ($\sqrt{3}$ times greater for crystal B) and the ω_{\max}^2 ($\omega_{\max B}^2 = 3 \omega_{\max A}^2$).

With equations (23) and (22) in equation (14) we get the velocity-stress relation for a dislocation moving in a random alloy of isotopic defects with concentration C_B

$$\frac{\sigma(C_B)}{\mu} = 4 \pi \int_{-\pi}^{\pi} dK_x P \int_{-\infty}^{\infty} dK_y \frac{\sin^2 K_x/2}{K_y} \times \left\{ 4 \left[\sin^2 \frac{K_x}{2} + \sin^2 \frac{K_y}{2} \right] + \frac{C_B M_A \varepsilon \left(\frac{v}{c}\right)^2 K_y^2}{1 - (1 - C_B) M_A \varepsilon \left(\frac{v}{c}\right)^2 K_y^2 P_{zz}^{00} \left[\left(\frac{v}{c}\right)^2 K_y^2 \right]} - \left(\frac{v}{c}\right)^2 K_y^2 - i\Gamma K_y \right\}^{-1} \quad (24)$$

The numerical evaluation of equation (24) requires the three-dimension integral $P_{zz}^{00} \left[\left(\frac{v}{c} K_y \right)^2 \right]$ which explicitly reads :

$$P_{zz}^{00} \left\{ \left(\frac{v}{c} \right)^2 K_y^2 \right\} = \sum_{\sigma} \frac{b^3}{(2\pi)^3} \int_{BZ} d^3k \frac{1}{M_A \{ \omega^2(k, \sigma) - (vk_y)^2 - i\Gamma k_y \}}. \quad (25)$$

Numerical evaluation of (24) for $C_B = 0.25, 0.5$ and 1 is shown in figures 4, 5 and 6.

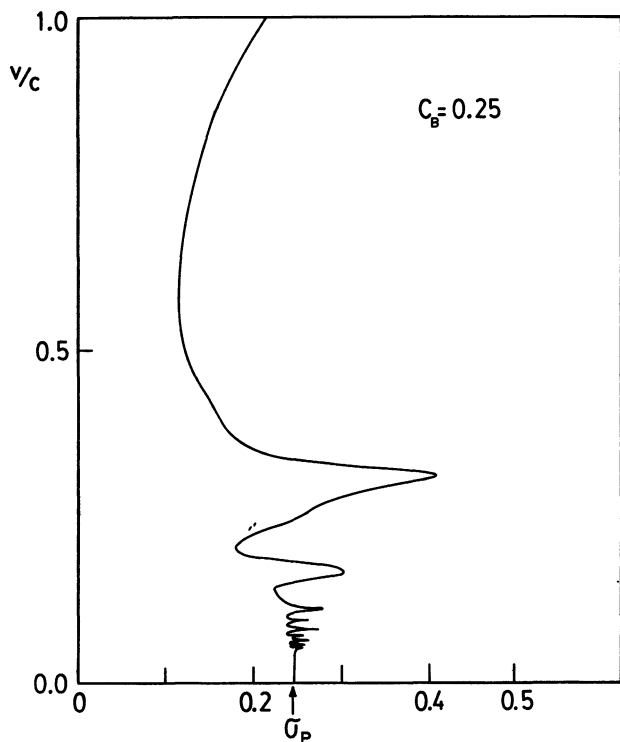


Fig. 4. — Dislocation velocity (divided by sound velocity), v/c , versus applied shear stress (divided by shear modulus), σ/μ , for a screw dislocation moving uniformly in a simple cubic lattice (atomic mass M_A containing a random array of mass-defects (mass $M_B = M_A/3$) of concentration $C_B = 0.25$).

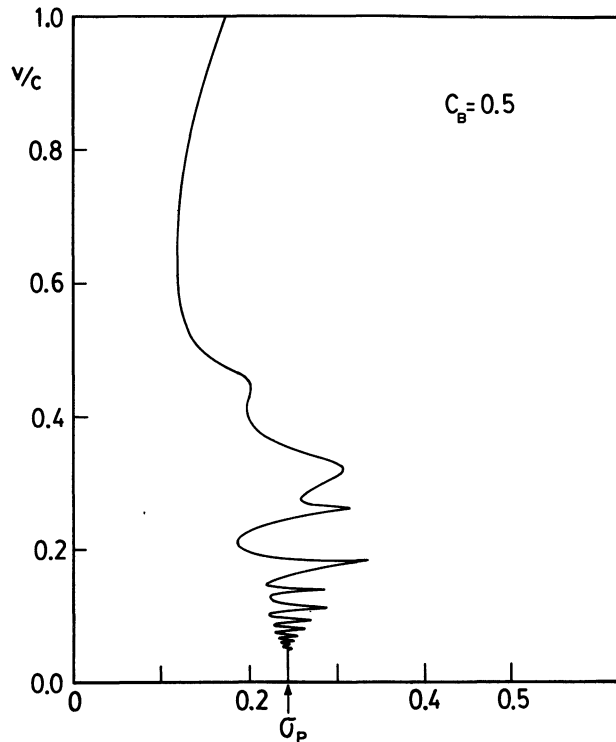


Fig. 5. — Same as figure 4 except $C_B = 0.5$.

minimum stress as a function of velocity (appearing for velocities equal to $\approx 0.5 c$ for $C_B = 0$; $\approx 0.6 c$ for $C_B = 0.5$ and $\approx 0.8 c$ for $C_B = 1$) is constant $\sigma_{\min} = 0.11 \mu$ independent of the concentration.

Several important features stand out from these figures. First, for very low velocities, $v = 0.05 c$ any effect of the mass-defects disappears; in particular the value of σ_p is not a function of the concentration. This fact is intuitively evident, since at very low velocities the inertial effects should be negligible. For the intermediate velocities, as the concentrations C_B or C_A approach the value $1/2$ the divergences in the stress disappear as a consequence of the damping of phonons. Finally at high velocities the light defects soften the crystal (the stress necessary to move a dislocation at a given velocity appears to be a decreasing function of the concentration of the light element). For example for $v/c = 1$ we find $\sigma = 0.28 \mu$ for $C_B = 0$, $\sigma = 0.20 \mu$ for $C_B = 0.25$ and $\sigma = 0.15 \mu$ for $C_B = 0.5$. But it is interesting to note that the

3. Discussion and conclusions.

A point defect described within the framework of elasticity theory may only harden a crystal (by reducing the dislocation mobility), regardless of whether the interaction energy is positive or negative. Also, a mass-defect does not interact with a dislocation in that theory.

In this work it is shown how point defects can be introduced in a lattice-dynamics model of a moving dislocation. Calculations have been made for a mass-defect because of its simplicity — diagonal disorder. Despite this simplicity, the model allows us to see, at least in a general way, what new effect may be associated with a mass-change. By introducing a general force-constant *and* mass defect, we should be

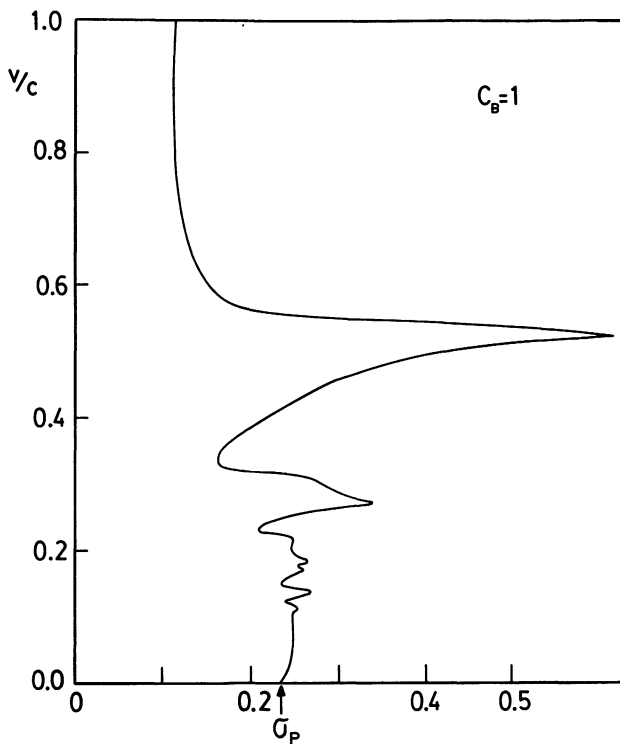


Fig. 6. — Same as figure 4, except $C_B = 1$.

able, in the future, to describe the equivalent to the inhomogeneity interaction of continuum theory and the effects of the mass change at the same time. Finally it should be possible to introduce an additional Kanzaki force to describe point defects with size misfit; then a complete description of all possible interactions should be achieved, not only for the

calculation of the Peierls stress but for the entire dynamic range.

An important consequence of this formalism is that it allows a description of the two types of possible modifications of the dislocation mobility due to the presence of point defects, hardening and softening. For instance, if a light isotopic defect increases the mobility at high velocities, a heavy defect decreases that mobility. This is important in the description of the peaks in those parameter associated with the dislocation mobility, like internal friction, as a function of defect concentration [15, 16].

In a further degree of sophistication of the model, it should be possible to introduce point defects in interstitial positions. In the case of the dumbbell interstitial in f.c.c. lattices, the low frequency resonances produced by the librational and translational modes [17] could have interesting consequences on the dislocation mobility as mentioned in reference [7].

Finally the inverse problem can be studied. A moving dislocation radiates transverse phonons with a frequency distribution which is a function of its velocity and the model parameters. A point defect having peaks in its local frequency spectrum at those particular frequencies could be excited at high amplitudes. If the vibration corresponds to a diffusion mode the diffusion coefficient could be modified in the neighbourhood of a moving dislocation.

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