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The Distribution of Vacancies and Hard Impurity Atoms around an Edge Dislocation

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The form and magnitude of the size effect interaction and the second order inhomogeneity effect interaction between a point defect and an edge dislocation are discussed. It is shown that, by taking both these interactions simultaneously into account, the binding energy between a relatively hard impurity atom and a dislocation can be estimated without introducing the usual arbitrary cut off near the dislocation core. Furthermore, such impurities should form a displaced Maxwellian atmosphere with a bounded maximum concentration beneath the edge dislocation.

The second order inhomogeneity interaction is used to calculate the kinetics of vacancy annealing. The predicted kinetics differ from the previous published theoretical results.

The elastic interaction between a point defect and a line dislocation can be separated into two distinct contributions: a) an interaction E_1 arising from the difference in size between solute and solvent atoms, b) a second order interaction E_2 which appears if the solute atoms behave like a small region with different elastic constants from those of the matrix crystal¹⁾.

By replacing the solute atom of radius $r_0(1+\delta)$ by an elastic sphere of the same size and inserting this into a spherical cavity of radius r_0 , Eshelby²⁾ shows that

$$E_1 = -\delta \int_{V} p_{ii} dv \qquad (1)$$

where p_{ij} is the stress field of the dislocation and the integral is evaluated over the spherical volume $V=4/3 \cdot \pi r_0^3$. For an edge dislocation in an isotropic elastic medium, p_{ii} is a potential function and therefore we have the *exact* result¹:

$$E_1 = -\delta V p_{ii}(R, \phi) \tag{2}$$

where (R,ϕ) are the cylindrical polar coordinates of the center of the spherical inclusion with the dislocation lying along the z axis. In a previous analysis Bilby³⁾ gives the erroneous impression that (2) is an approximate result valid only to $0(r_0/R)^2$. Thus we obtain the well-known result, in the usual notation

$$E_{1} = \frac{(1+\nu)\mu \, b \, V \, \delta \sin \phi}{\pi (1-\nu) \, R} \, . \tag{3}$$

and the surrounding matrix has been considered by Eshelby²⁾. The solute atom is replaced by an equivalent elastic inclusion and a general expression for this second order interaction energy is developed. In particular it may be shown that near an edge dislocation situated as above

$$E_{2} = \frac{15}{8\pi^{2}(1-\nu)(4-5\nu)} \frac{\mu b^{2} V}{R^{2}} \times \left[1 + \frac{2(1-12\nu+10\nu^{2})\sin^{2}\psi}{5}\right] \quad (4)$$

for an infinitely hard spherical atom and

$$E_{2} = -\frac{15}{4\pi^{2}(1-\nu)(7-5\nu)}\frac{\mu b^{2} V}{R^{2}} \times \left[1 - \frac{(1+6\nu-5\nu^{2})\sin^{2}\psi}{5}\right]$$
(5)

for a spherical void $(vacancy)^{4}$.

Eq. (4) shows a net repulsion from the edge dislocation which is greatest perpendicular to the slip plane ($\phi = \pm \pi/2$), whereas Eq. (5) shows a net attraction which is greatest on the slip plane ($\phi = 0$).

The total elastic interaction energy E_{τ} between an edge dislocation and a hard solute atom is thus given by the sum of E_1 and E_2 given by Eq. (4). Thus E_T has a bounded maximum negative value of

$$E_{T(MAX)} = -3.4\mu V\delta^2 \tag{6}$$

at the position

r

$$=0.3b/\pi\delta, \ \phi = -\pi/2 \tag{7}$$

The interaction E_2 arising from a difference with Poisson's ratio equal to 1/3. Conin elastic constants between the solute atom sequently the formation of a displaced Maxwellian atmosphere is possible in this case without account being taken of the detailed dislocation core configuration; that is no arbitrary cut-off of the elastic interaction energy E_1 is necessary. Such a displaced atmosphere in low carbon and nitrogen steels could conceivably become ordered near the dislocation and lead to the formation of a local martensitic phase; precipitates with a martensitic structure associated with dislocations in α -iron have been identified by reflection electron diffraction by Doremus and Koch⁵⁾ and similar ribbon-like precipitates slightly displaced from the dislocation lines have been observed by transmission electron microscopy by Fisher⁶⁾.

The interaction energy between a lattice vacancy and an edge dislocation primarily consists of E_2 , given by Eq. (5). It is interesting to note that the binding energy on the plane adjacent to the slip plane is approximately twice Friedel's estimate⁷ which neglected the shear field of the dislocation⁴. The fact that the binding energy is a maximum on the slip plane, with the consequent enhanced vacancy concentration there, may be important in the process of cleavage fracture when the cleavage plane coincides with the primary slip plane (zinc, silicon, for example).

When vacancies are in supersaturated solution in a crystal they will be attracted to the dislocations which can act as sinks for their annihilation. Due to the short range nature of the interaction the concentration gradients away from the dislocations will be everywhere small which allows diffusion flow to be neglected, in contrast to the analogous pure drift flow analysis of Cottrell

and Bilby^{8),9)} for the size effect interaction where persistent infinite concentration gradients are produced. The kinetics of this annealing process have been calculated by Friedel assuming a purely radial interaction potential. We have extended this to take account of the angular term in Eq. (5). It can be shown that, starting from an initially uniform concentration C_0 , the number of vacancies N(t) that arrive at unit length of an isolated edge dislocation in time t is given by

$$N(t) = 7.79 C_0 \left[\frac{A D t}{kT} \right]^{1/2}$$
 (8)

where D is the diffusion coefficient, T is the absolute temperature, k is Boltzmann's constant, $A=15\mu b^2 V/4\pi^2(1-\nu)(7-5\nu)$ and $\nu=1/3$. The time dependence is thus the same as obtained by Friedel⁷ but N(t) is approximately double his value.

References

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DISCUSSION

Koehler, J. S.: Can you tell us the relative magnitudes of the interaction E_1 and E_2 for a vacancy at about ten atomic distances from the dislocation?

Bullough, R.: In the calculation of the vacancy annealing kinetics we have ignored any size-effect contribution to the interaction energy. That is, we have neglected the strain field of the isolated vacancy and treat it as a simple soft spot in the crystal. However, if the radial strain associated with the vacancy is $\delta \delta_{ij}$, then at 10*b* from the dislocation, $E_1 \simeq -10^{-1} \mu V \delta$ and $E_2 \simeq -10^{-3} \mu V \delta$. Thus E_1/E_2 (at r=10b) $\simeq 100\delta$. They are therefore comparable for a 1% strain. The ratio E_1/E_2 , however, decreases rapidly with distance from the core.

Otte, H. M.: Could you explain what you mean by a martensitic structure? Do you have in mind a structure formed martensitically? If this is so, then, since you

are discussing Fe already in the body centered cubic form, do you suggest that regions of tetragonal martensite form or that an Fe carbide forms? If this formation is indeed martensitic, can you predict a macroscopic shear for the reaction?

Bullough, R.: When I used the term martensitic structure, I was not implying anything about its mode of formation. I simply meant that precipitates near an edge dislocation with a body centred tetragonal martensite structure should suffer a localized repulsion from the edge dislocation.

Kuhlmann-Wilsdorf, D.: While your calculation on the attraction of vacancies to edge dislocations due to their interaction with shear stresses coincides with our own (lecture I F 12)* everywhere outside of the dislocation cores, it cannot be applied inside of them. (For typical close-packed metals the critical distance is $r \leq 6b$). The reason for this is that the shear stress on the slip plane cannot possibly rise beyond the critical shear stress of an ideal crystal, which value is reached at the rim of the core. On the other hand, normal stresses, absent on the slip plane of an edge dislocation outside of its core, are very strong and definitely dominant inside of the core. Even though the linear distances of relaxation of the first neighbor shell to a vacancy was calculated to only a few percent of normal distances by Girifalco, this does not mean that the vacancy relaxation volume is small. In fact, since the first shell in close packed metals includes a total volume of about 13v, with v the atomic volume, the calculated linear distances of relaxation correspond to a volume of relaxation of $\simeq 2v/3$. For the purposes of the present calculation, the outward relaxation volume of the second shell must be subtracted from this figure, the inward relaxation of the third shell be added, and so on. According to present best evidence available, this sum converges very rapidly to a value of about 0.5v. Therefore, the volume effect is far from negligible, but instead is several times larger than the interaction between vacancies and shear stresses. For this reason, in metals the vacancies will not aggregate along the slip plane in the core of edge dislocation. Incidentally, the formula given for E_{int} can be greatly simplified, as is explained in our own paper (lecture I F 12)* and, more completely, in a detailed publication to appear within the next several months.

* Proc. Int. Conf. Cryst. Latt. Def. (1962): J. Phys. Soc. Japan 18 Suppl. II (1963) 230.

Bullough, R.: In our treatment of the vacancy interaction we have replaced the vacancy by a spherical void in an elastic continum and have assumed that the dominant interaction with a dislocation is the inhomogeneity interaction. Clearly, if there is a large radial strain associated with a vacancy in the face-centred cubic metals then the first order elastic interaction should also be taken into account (see reply to Professor Koehler). However, the observations of $t^{1/2}$ vacancy annealing kinetics in such metals can be interpreted (as we show in our paper) by assuming a dominant inhomogeneity interaction and do not follow if a large size effect contribution is allowed for. In your treatment of the problem (paper I F 12)*, you also introduce a further second order interaction arising from the interaction of the vacancy strain with the local vibrational modes of the crystal. I am surprised that with your adoption of a large vacancy relaxation that this second order contribution is comparable to the first order size effect interaction and is sufficient to inhibit climb processes at high temperatures. Also I feel that the use of a core radius of 6b is questionable. The half width of the Peierls edge dislocation is 0.75b and I would think, therefore, that our cut off radius of r=b was not unreasonable.