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POINT DEFECT DISLOCATION INTERACTION IN A CRYSTAL UNDER TENSION

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INTERACCION ENTRE UN DEFECTO PUNTUAL Y UNA DISLOCACION EN UN CRISTAL TENSIONADO

Se estudia teoricamente la influencia de una tensión uniaxial externa en la interacción entre defectos móbiles y dislocaciones de la red. Los defectos puntuales se describen utilizando el formalismo de función de Green de la red. La energía de interacción con una fuente de tensiones internas es deducida. Se calcula la energía correspondiente a la interacción entre defectos puntuales intrínsecos y una dislocación en un cristal cúbico centrado en las caras sometido a tensiones. El propósito del trabajo es realizar un análisis crítico de las bases de la teoría de "creep" bajo irradiación que explica el fenómeno a través de una atracción preferencial de los intersticiales y vacancias hacia dislocaciones con cierta orientación respecto al eje externo de tensión. La atracción hacia dislocaciones de borde se discute usando una expresión que incluye el carácter discreto de la difusión del defecto en la red. Se concluye que el proceso de creep bajo irradiación enunciado anteriormente sólo tendrá lugar si los tensores dipolares de los auto-defectos en la configuración de equilibrio y la activada cumplen ciertas relaciones definidas.

POINT DEFECT DISLOCATION INTERACTION IN A CRYSTAL UNDER TENSION

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The influence of an external uniaxial stress on the interaction between mobile defects and individual network dislocations is theoretically studied. The point defects are described within the lattice Green's function formalism. Their interaction energy with a source of internal stress is deduced. This energy is calculated between intrinsic point defects and a dislocation in a strained f. c. c. crystal. The work aims at examining the foundations of the irradiation creep theory that explains the phenomenon as a preferential drift of interstitials and vacancies to dislocations with particular orientations to the external stress axis. The drift to edge dislocations is discussed using an expression that includes the discrete character of the jump. It is concluded that the proposed model of irradiation creep can only be sustained if the dipole tensors of the defects at the equilibrium and saddle point configurations fulfill some specific relations.

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1. Introduction

In recent publications (Heald and Speight, 1974 a), 1974 b), 1975; Bullough and Willis, 1975; Bullough, 1975), it has been suggested that the irradiation creep measured in nuclear materials is attributable to the preferential drift of irradiation produced point defects towards network dislocations. Heald and Speight- (1974 a), (1974 b)- (henceforth referred to as HS) conjectured that edge dislocations with their Burgers vector parallel to a tensile stress will climb through a bias interstitial absorption, whereas those with this vector perpendicular to the stress will attract preferentially vacancies with respect to interstitials. These authors modelled the point defect as a spherical inhomogeneity. This is distorted by the applied stress and a preferential interaction between the point defect and the favourably oriented dislocation is induced. In order to check the validity of HS's assumptions Bullough and Willis (1975) (henceforth referred to as BW) performed an elastic calculation of the stress induced interaction energy between a dislocation and a point defect modelled as a spherical inclusion. The difference in linear response in the vicinity of the defect with respect to the perfect matrix was introduced by allowing the elastic constants of the inclusion to differ from the matrix constants. BW found particular preferences in the interaction energy and concluded that those support the creep mechanism proposed by HS. More recently, Bullough (1975) reviewed this mechanism and compared it with experimental results; this author concludes that it provides the dominant contribution to the low temperature irradiation creep.

The purpose of the present paper is to include the discrete nature of the lattice in the study of the interaction between point defects and dislocations in presence of an external stress and the resultant defect drift towards the dislocation sinks. In the next section we deduce a general expression for the elastic interaction energy between a lattice point defect and a source of internal strain in the crystal. We, then, briefly summarize some of the present knowledge of the intrinsic point defects symmetry in a f. c. c. lattice. The expression for the interaction energy plus the general symmetry of the defects are used to repeat BW's calculations of the interaction between a dislocation and a point defect in the framework of a discrete model for the defect. In Section 3 we study the diffusion of anisotropic point defects in a field of force. The validity of Kronmüller, Frank and Hornung's approach (1971) is asserted and clarifying examples are solved. Finally the feasability of HS mechanism of creep in a f. c. c. crystal is discussed. It is concluded that a creep process by preferential absorption of irradiation produced defects at different network dislocations can only be sustained if allowed by the symmetry of the defect at the equilibrium and saddle point configurations. Though the immediate interest of the work is HS's irradiation creep model, the expressions for the interaction energy and drift of point defects towards internal sinks are deduced and studied under a general format.

2 a) Interaction energy between a point defect and a strain field

Eshelby (1951) proved that, given a system of internal stress S, whose sources lie entirely within a surface Σ, and another system T, whose sources lie entirely outside Σ; their elastic interaction energy is given by the volume integral:

$$E_{int}(S,T) = -\int \underline{f}^S \cdot \underline{u}^T \, dv \qquad (1)$$

taken over the interior of Σ. Where $\underline{f}^S$ is a fictitious distribution of body forces inside Σ that produces the same stress on and outside Σ as does the actual source of internal stress within Σ. We will find the corresponding forces considering a dis - crete model for the point defect, taken as the system S. The integral in eq. (1) must be replaced by a summatory over lattice points.

Given the point defect S we consider its core enclosed by the surface Σ, far enough to approximately satisfy the equation:

$$\underline{u}^S_{\Sigma} = \underline{\underline{\varepsilon}}^S \underline{x}^0 \qquad (2)$$

in absence of other strain source in the crystal, where $\underline{\underline{\varepsilon}}^S$ is a homogeneous strain field and $\underline{x}^0$ the perfect lattice position. It is also assumed the displacements due to the interacting defect or source of internal stress T (it can be an external applied stress) to have an equivalent expression on and within Σ:

$$\underline{u}^T = \underline{\underline{\varepsilon}}^T x^0 \qquad (3)$$

Then, in order to calculate the interaction energy the atomic configuration of a block Σ, containing the defect S, must be solved with boundary conditions:

$$\underline{u}_{\Sigma} = (\underline{\underline{\varepsilon}}^T + \underline{\underline{\varepsilon}}^S)\, x^0 \qquad (4)$$

Once the displacements $\underline{u}^S$, solution of the problem within Σ, are found, the forces $\underline{f}^S$ - eq. (1) - correspond to the Kanzaki forces (1957), defined as:

$$\underline{f}^S = \underline{\underline{\Phi}}^0 \, \underline{u}^S \qquad (5)$$

where $\underline{\underline{\Phi}}^0$ is the perfect lattice force constants matrix.

Dederichs, Lehman and Sholz (1975) performed an equivalent calculation to find the change of the crystal elastic constansts due to a dumbbell interstitial in copper. They calculated the displacements $\underline{u}^S$ by computer simulation of a block of atoms interacting via a short range potential.

The interstitial was located at the center of the block and the homogeneous displacements due to an external stress field imposed over the boundary atoms. If those atoms had remained at the perfect lattice position a set of Kanzaki forces $\underline{f}^{0S}$ - eq. (5) - would have been obtained. The effect of the boundary displacements can be introduced through a change on those forces:

$$\delta \underline{f} = - \underline{\underline{t}} \cdot \underline{u}_{\Sigma} \quad , \qquad (6)$$

where the matrix t has been defined by Dederichs et al. (1975). The Kanzaki forces corresponding to the boundary conditions (4) are:

$$\underline{f}^{S} = \underline{f}^{0S} + \delta \underline{f} = \underline{f}^{0S} - \underline{\underline{t}} \cdot (\underline{\underline{\xi}}^{S} + \underline{\underline{\xi}}^{T}) \cdot \underline{x}^{0} \quad . \qquad (7)$$

Replacing eqs. (3) and (7) in eq. (1) we obtain the interaction energy:

$$E_{int}(S,T) = -\sum (\underline{f}^{0S} - \underline{\underline{t}} \cdot \underline{\underline{\xi}}^{S} \cdot \underline{x}^{0} - \underline{\underline{t}} \cdot \underline{\underline{\xi}}^{T} \cdot \underline{x}^{0}) \cdot \underline{\underline{\xi}}^{T} \cdot \underline{x}^{0} =$$

$$= - \sum \tilde{\underline{f}}^{S} \cdot \underline{\underline{\xi}}^{T} \cdot \underline{x}^{0} + \sum \underline{\underline{t}} \cdot (\underline{\underline{\xi}}^{T} \cdot \underline{x}^{0})^{2} , \qquad (8)$$

where the summatory is taken over the lattice sites within Σ and the forces $\tilde{\underline{f}}^{S}$ are the Kanzaki forces corresponding to a single defect S in an infinite crystal. The first term in equation (8) corresponds to the first order, size interaction energy and the second to the induced, second order interaction. This last term arises because the lattice response to an applied stress in the vicinity of the point defect differs from the response in the perfect, defect free, matrix.

Equation (8) can be explicitly developed if the defect S is assumed to be "soft". This means it is modelled through a set of forces applied over near neighbours host atoms and a harmonic response of the host lattice, in agreement with Tewary's static Green's function method (1973). The displacement field due to the defect results:

$$\underline{u}^{S} = \underline{\underline{G}}^{0} \, \underline{f}^{*S} \quad , \qquad (9)$$

where G^{0} is the perfect lattice Green's function (Tewary, 1973; Schober, Mostoller and Dederichs, 1974) and $\underline{f}^{*S}$ are the forces obtained from the derivatives of the defect-host atom interatomic potential at the final, relaxed positions:

$$f_i^{*S} = - \left. \frac{\partial V^{S-a}}{\partial x_i} \right|_{\underline{x}_a = \underline{x}_a^{0} + \underline{u}_a} \quad . \qquad (10)$$

In this approximation:

$$\tilde{\underline{f}}^{S} = \underline{f}^{*S}$$

and

$$t_{ij} = -\partial f_i^{*S} / \partial x_j = \left. \frac{\partial^2 V^{S-a}}{\partial x_i \partial x_j} \right|_{\underline{x}_a = \underline{x}_a^0 + \underline{u}_a} \qquad (11)$$

The anisotropy of the defect is important for both terms in eq. (8). This is reflected in the defect dipole tensor, defined as:

$$p_{ij} = \sum_{\underline{l}} \tilde{f}_i^S (\underline{l})\, x_j^0 (\underline{l}) \qquad (12)$$

and in a higher order, polarizability tensor:

$$\Phi_{ijkl} = \sum_{\underline{l}, \underline{l}'} t_{ij} (\underline{l}, \underline{l}')\, x_k^0 (\underline{l})\, x_l^0 (\underline{l}') \qquad (13)$$

2 b) Dipole tensor for the vacancy and interstitial in a f. c. c. lattice

Some dipole tensor values - eq. (12) - for a vacancy and a dumbbell interstitial in a f. c. c. lattice are reported in Table I. Those were obtained by using different interatomic potentials fitted to copper parameters and the tensors corre - sponding to the equilibrium and saddle point configurations are reported. In the same table values obtained in the, called by us, soft point defect approximation appeared. There, the defect-host atom force defined by eq. (10) was used. The point defect configurations were obtained from Johnson's computer simulation results (Ref. Girifalco and Welch, 1967) and from Tewary's calculation (1969) . The last was performed by using the perfect lattice Green's function constructed with Born Von Karman boundary conditions and evaluating the forces in the harmonic approximation. In Table I the eigenvalues of the dipole tensor are reported in the symmetry directions.

From Table I it is seen that, though the tensor eigenvalues as well as their ratio depend on the interatomic potentials and the defect model, a general pat_ tern appears, related to the symmetry of the lattice and the point defect.

We will summarize the general shape of the dipole tensors for the va- cancy and the dumbbell interstitial. The cartesian axes will be taken as perpendicular to the crystallographic axes. The vacancy at its equilibrium configuration results, fully symmetric:

$$p_{ij}^V = -\lambda \delta_{ij} \qquad (14)$$

On the contrary the saddle point configuration for a jump to a near neighbour posi- tion is strongly anisotropic. From figure 1 we see it corresponds to two vacant sites with an interstitial atom midway. That interstitial imposes a large dilatation

field, pushing outwards the four near neighbour atoms. The dipole tensor resutls, approximately:

$$P_{ij}^{\binom{VS}{110}} = \begin{vmatrix} g_1 & -g_{12} & 0 \\ -g_{12} & g_1 & 0 \\ 0 & 0 & g_3 \end{vmatrix} , \qquad (15)$$

where $g_3 \gg g_1$ and a jump from the origin to the neighbour (110) lattice site is considered.

For the (100) dumbbell interstitial the dipole tensor eingenvalue is larger in the directions perpendicular to the interstitial axis than in the parallel one. Then:

$$P_{ij}^{(100)} = \begin{vmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_2 \end{vmatrix} , \qquad (16)$$

where $\lambda_2 > \lambda_1$. The interstitial saddle point configuration (figure 1) shows a larger distortion in the direction normal to a plane determined by the dumbbell symmetry axis before and after the jump than in those contained in the plane. The dipole tensor has a symmetry similar to that corresponding to the vacancy saddle point:

$$P_{ij}^{\binom{100}{110}} = \begin{vmatrix} g_1 & g_{12} & 0 \\ g_{12} & g_1 & 0 \\ 0 & 0 & g_3 \end{vmatrix} , \qquad (17)$$

where $g_3 > g_1$ and the subscripts (100, 110) correspond respectively to the initial orientation of the interstitial and the final position after the migration jump, taking the origin at the initial location.

2 c) Point defect-straight dislocation interaction energy in a crystal under uniaxial tension

Following BW we shall study two cases;

I: the applied uniaxial external stress τ is parallel to the Burgers vector $\underline{b}$ of the edge dislocation;

II: τ is perpendicular to $\underline{b}$ (figure 2). The direction of the Burgers vector will be always taken as the x_1 axis. Assuming that the defect dipole tensor can be expressed as:

$$P_{ij} = \alpha_1 \delta_{ij} , \qquad (18)$$

we will calculate its interaction energy with the straight dislocation. It is also

assumed that the strain (3) on and within the volume Σ containing the defect is given by the addition of the dislocation and external strain fields:

$$\underline{\underline{\varepsilon}}^{T} = \underline{\underline{e}}^{D} + \underline{\underline{\varepsilon}}^{ext} \quad , \qquad (19)$$

where $\underline{\underline{e}}^{D}$ is taken as constant within Σ and equal to the value at the center of the block.

Assuming a elastic isotropic medium the strain field due to the applied stress results in case I:

$$\varepsilon_{11}^{ext} = \varepsilon, \varepsilon_{22}^{ext} = \varepsilon_{33}^{ext} = -\nu\varepsilon, \varepsilon_{ij}^{ext} = 0 \quad \text{if } i \neq j \qquad (20)$$

and in II:

$$\varepsilon_{11}^{ext} = \varepsilon_{33}^{ext} = -\nu\varepsilon, \varepsilon_{22}^{ext} = \varepsilon, \varepsilon_{ij}^{ext} = 0 \quad \text{if } i \neq j, \qquad (21)$$

If only those terms linear in the dislocation and external strain fields are included, the interaction energy between the dislocation and external strain fields and the point defect - eq (8) - is composed by three terms, two of those dependent on the dislocation field $\underline{\underline{e}}^{D}$. The interaction energy between the defect and the dislocation is given by those two terms. They are respectively the first order, size interaction and the second order, stress induced interaction. Then, in case I:

$$E_{int}^{I}(p.d., D) = -\alpha_1 e_{11}^{D} - \alpha_2 e_{22}^{D} + \varepsilon e_{11}^{D} \underline{\underline{\Phi}}_{1111} -$$

$$-\nu\varepsilon e_{22}^{D} \underline{\underline{\Phi}}_{2222} + \varepsilon e_{22}^{D} \underline{\underline{\Phi}}_{1221} - \nu\varepsilon \left[e_{11}^{D} (\underline{\underline{\Phi}}_{1221} + \underline{\underline{\Phi}}_{1331}) + e_{22}^{D} \underline{\underline{\Phi}}_{2332} \right]$$

(22)

and in II:

$$E_{int}^{II}(p.d., D) = -\alpha_1 e_{11}^{D} - \alpha_2 e_{22}^{D} - \nu\varepsilon e_{11}^{D} \underline{\underline{\Phi}}_{1111} + \varepsilon e_{22}^{D} \underline{\underline{\Phi}}_{2222} -$$

$$- \nu\varepsilon e_{11}^{D} \underline{\underline{\Phi}}_{1331} - \nu\varepsilon e_{22}^{D} (\underline{\underline{\Phi}}_{2112} + \underline{\underline{\Phi}}_{2332}) + \varepsilon e_{11}^{D} \underline{\underline{\Phi}}_{1221} , \qquad (23)$$

where p.d. stands for point defect, D for dislocation and $\underline{\underline{\Phi}}$ has been defined in eq.(13).

In Table I we have reported some values of the vacancy dipole tensor for copper. The polarizability tensor $\underline{\underline{\Phi}}$ - eq. (13) - is calculated in the soft point defect

approximation - eq. (11) - using Tewary's configuration for the vacancy in copper (Tewary, 1969). The following relations result:

$$\Phi^V_{1111} = \Phi^V_{2222} \; , \; \Phi^V_{2112} = \Phi^V_{1221} = \Phi^V_{1331} = \Phi^V_{2332}$$

and (24)

$$\text{sign}\,(p^V_{ii}) = \text{sign}\,(\Phi_{1111}) = \text{sign}\,(\Phi_{1221}) \quad .$$

The last set of relations is also necessary for the vacancy to provide a negative contribution to the average crystal rigidity and shear modulus, in agreement with BW's assumption.

If the values of the vacancy dipole tensor - eq. (14) - and the relations (24) are replaced in eqs. (22) and (23), the point defect-dislocation interaction energy values for both orientations of the applied stress can be compared (figure 2). This comparison will determine the existence of a preferential attraction dependent on the stress orientation. BW performed the same calculation but modelling the defect as a spherical inhomogeneity. Isotropic elasticity is used to describe the dislocation field since Tomé and Savino (1976) have shown that the main anisotropic effects in the interaction are related to the point defect configuration. The average value is considered for the dislocation field; it means in the equations for the dislocation strain field (Nabarro, 1967) x_1^2 / r^2 and x_2^2 / r^2 are replaced by their mean value 1/2 (BW). Then, the amplitudes of the interaction energies (22) and (23) for the vacancy case result:

$$\mathcal{A}\left[E^I_{int} (v, D) \right] = \frac{b}{2\pi r} \left\{ |\alpha| \, \frac{(1 - 2\nu)}{(1 - \nu)} - \frac{\varepsilon (1 - \nu + \nu^2)}{(1 - \nu)} \left| \Phi_{1111} \right| + 3\nu\varepsilon \left| \Phi_{1221} \right| \right\} \qquad (25)$$

and

$$\mathcal{A}\left[E^{II}_{int} (v, D) \right] = \frac{b}{2\pi r} \left\{ |\alpha| \, \frac{(1 - 2\nu)}{(1 - \nu)} + \frac{\varepsilon\nu (2 - \nu)}{(1 - \nu)} \left| \Phi_{1111} \right| - \frac{\varepsilon (1 - 2\nu + 3\nu^2)}{(1 - \nu)} \left| \Phi_{1221} \right| \right\} \qquad (26)$$

We substract (26) from (25) to obtain:

$$\mathcal{A}\left[E^I_{int} (v, D) \right] - \mathcal{A}\left[E^{II}_{int} (v, D) \right] = - \frac{\varepsilon b (1 + \nu)}{2\pi r (1 - \nu)} \left[\left| \Phi_{1111} \right| - \left| \Phi_{1221} \right| \right] \qquad (27)$$

Our calculation of the polarizability tensor - eqs. (11) and (13)-results in $|\Phi_{111}|$ bigger than $|\Phi_{1221}|$ ($\Phi_{1111} = -23.2$ eV, $\Phi_{1221} = -13.8$ eV). Therefore a vacancy results preferentially attracted by an edge dislocation with its Burgers vector perpendicular to the applied stress. This result, obtained in an independent way, agrees with BW conclusions. Both calculations are based on a set of compatible assumptions with respect to the structure of the vacancy in a f. c. c. lattice and its interaction with a dislocation.

The interstitial is in general more anisotropic than the vacancy. The three possible orientations of the dumbbell interstitial may have a different interaction energy with the dislocation. Assuming that the Burgers vector of the edge dislocation (figure 2) agrees with a (100) crystallographic direction, the amplitudes of the first order interaction energies between different orientations of the interstitial and the average dislocation field are:

$$\mathcal{A}\left\{E_{int}\left[(100)\ d.b.,\ D\right]\right\} = \left|\alpha_1\ \bar{e}^{d}_{11} + \alpha_2\ \bar{e}^{D}_{22}\right| = \frac{b}{2\pi r}\left|\lambda_1 - \lambda_2\ \frac{\nu}{1-\nu}\right|$$

$$\mathcal{A}\left\{E_{int}\left[(010)\ d.b.,\ D\right]\right\} = \left|\alpha_2\ \bar{e}^{D}_{11} + \alpha_1\ \bar{e}^{D}_{22}\right| = \frac{b}{2\pi r}\left|\lambda_2 - \lambda_1\ \frac{\nu}{1-\nu}\right|$$

$$\mathcal{A}\left\{E_{int}\left[(001)\ d.b.,\ D\right]\right\} = \left|\alpha_2\ \bar{e}^{D}_{11} + \alpha_3\ \bar{e}^{D}_{22}\right| = \frac{b}{2\pi r}\ \lambda_2\ \frac{(1-2\nu)}{(1-\nu)}, \qquad (28)$$

where eq. (16) has been used. These terms are $1/\varepsilon$ times greater than the external stress induced interaction energy. The relative difference in energy between the different orientations of the dumbbell is given by the difference among the eigenvalues of the dipole tensor.

The external stress induced interaction energy between the interstitial and an edge dislocation is quite difficult to discuss in a general framework. Numerical calculations, similar to those of Dederichs et al. (1975), should be done with appropiate boundary conditions. The soft point defect approximation we used for the vacancy is not valid for the interstitial. We have found that, if the change in the crystal elastic constants due to the defect is determined in this approximation, relaxation of the atoms that constitute the dumbbell must be allowed in order to obtain the same trend in the results as Dederichs et al. (1975). We can approximately infer the polarizability tensor either from the change in elastic constants obtained by those authors or from the soft point defect approximation allowing the dumbbell atoms to relax. Through these approximations we arrive to the apposite conclusion than the one of BW for the interstitial case. It means, we find the interstitial to be preferentially attracted by the dislocation in case II with respect to I (figure 2). However the fact that the $\underline{t}$ matrix of eq. (6) depends on boundary conditions must be allowed for.

3 a) Drift of point defects in a field of force

The migration of point defects towards an individual crystal sink is influenced by their interaction energy-E_{int}- with it. This is the so called stress-assisted diffusion. In a continuum model the flux of mobile defects (p.d.) is given by (Heald and Speight, 1975):

$$\underline{J} = -\left[D \nabla C + \frac{DC}{KT} \nabla E_{int} (p.d., sink)\right] \qquad (29)$$

where D stands for diffusivity and C for concentration of point defects. Accepting this approximation, the eventual difference among the drift towards dislocations with different orientations in the stressed body is determined by the variation of the dislocation-point defect interaction energy as a function of that orientation. This is HS approximation to discuss the irradiation creep mechanism. In general the discrete character of the lattice imposes the point defect to have a lower symmetry than the perfect crystal and a finite number of feasible diffusion jumps. Girifalco and Welch (1967) and Kronmüller, Frank and Hornung (1971) have discussed the diffusion of anisotropic point defects in a field of forces and obtained an expression for the flux that converges in first order to eq. (29) but the second order terms result much more complex than the simple expansion of the interaction energy. Those depend on the symmetry of the point defect at the equilibrium and saddle point configuration.

In the following we shall use the fundamental equation for the current density of anisotropic point defects in a field of forces proposed by Kronmüller et al. (1971). In this approach the energy $E_i^{(n)}$, is defined as the potential energy of the lattice with the point defect at the equilibrium position " i " and its symmetry axis oriented in a " n " direction. The defect in order to jump from the position " i " with orientation " n " to a neighbour position " j" has to overcome a saddle point energy $Q_{ij}^{(n)}$. Then, the current density of defects at " i " is given by :

$$\underline{J}_i = \sum_{j \neq i}^{N} \sum_{n, n_{ij}} \left[\nu_{ij}^{\binom{n}{n_{ij}}} C_i^{(n)} - \nu_{ji}^{\binom{n}{n_{ij}}} C_j^{(n)} \right] \underline{S}_{ij} \quad , \qquad (30)$$

where $C_i^{(n)}$ is the density of defects at position " i " with orientation "n"; "N" the number of neighbour positions to " i " that can be occupied by one jump and the double summatory over n and n_{ij} runs overs all the possible orientations "n" and the number " n_{ij} " of single jumps from this orientation that result in a migration from "i" to "j". The jump frequency is given by:

$$\nu_{ij}^{\binom{n}{n_{ij}}} = \nu_{0_{ij}}^{(n)} \exp - \left(Q_{ij}^{\binom{n}{n_{ij}}} - E_i^{(n)} \right) / KT \quad . \qquad (31)$$

We shall consider in the applications that follow the preexponential factor to be constant ($\nu_{o\,ij}^{(n)} = \nu_o$). $\underline{S}_{ij}$ is the vector relating neighbouring positions "i", "j".

The potential energy of the lattice with the defect either at the saddle point or equilibrium configuration will be increased by the addition of the defect formation energy at that site plus its interaction with all other sources of stress in the crystal. We see in Eq. (31) that the interstitials and vacancies drift towards dislocations +) depends both on the interaction energy at equilibrium and at the saddle point configuration (the dipole tensor in both configurations having a different symmetry). If an external stress is applied the defect migration rate depends also on the first order dipole interaction with it and the drift of anisotropic point defects is modified in a very subtle way.

The equilibrium distribution is assumed for the defect orientations at a given site:

$$C_i^{(n)} = C_i \frac{\exp - E_i^{(n)}/KT}{\sum_n \exp - E_i^{(n)}/KT} \quad . \qquad (32)$$

This is a sound approximation when the rotation energy is smaller than the migration one. As discussed by Kronmüller et al. (1971), it should hold in general for times $t > \nu_{ij}^{-1}$, since the establishment of the orientational equilibrium requires only a few jumps. If Eqs. (31) and (32) are replaced in (30) and a Taylor expansion performed an expression similar to (29) results:

$$J_i = \sum_{j \neq i}^{N} \sum_{n, n_{ij}} \Big[\nu_o \, e^{-(Q_{ij}^{(n_{ij})} - E_i^{(n)})/KT}$$

$$\frac{C_i \, e^{-E_i^{(n)}/KT}}{\sum_m \exp - E_i^{(m)}/KT} - \nu_o \, e^{-(Q_{ij}^{(n_{ij})} - E_j^{(n)})/KT}$$

$$\frac{C_j \, e^{-E_j^{(n)}/KT}}{\sum_m \exp - E_j^{(m)}/KT} \simeq$$

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$$\simeq \; - \sum_{j \neq i}^{N} D_{ij} \left[\left(\underline{\nabla}_{ij} \, \bar{E} \right) C_i/KT + \underline{\nabla}_{ij} \, C_i \right] \qquad (33)$$

where

$$D_{ij} = \sum_{n, n_{ij}} e^{-(Q_{ij}^{(n_{ij})} - \bar{E})/KT} \, |S_{ij}|^2$$

$$\underline{\nabla}_{ij} A = \hat{S}_{ij} \cdot \underline{\nabla} A \; \hat{S}_{ij}$$

$$\bar{E} = -KT \ln \sum_{n} e^{-E_i^{(n)}/KT}$$

Eq. (33) reduces to the continuum approximation (29) if the migration energy is assumed to be independent of the jump direction ($Q_{ij}^{(n_{ij})} = Q_O^{(n)}$) and jumps into three orthogonal directions are considered. Eq. (29) contains only the first order terms for the flux of anisotropic defects in a field of forces. Therefore, the external stress induced drift towards a sink is not only determined by the effect of the stress on the interaction energy but also the local diffusivity (see Kronmüller et al. for definition) can be relevant. To show the influence of this parameter on the drift of anisotropic point defects we discuss in the next section the migration of a dipolar defect towards a dipolar sink in the presence of an external field. Afterwards more realistic and involved examples of defects in f. c. c. crystals are studied. The full Eq. (30) is used and the corresponding expansions indicated. Since we are only interested in the drift term a constant concentration of defect is considered ($C_i = C_o$).

3 b) Migration of a dipole towards a dipolar sink in presence of an external field

We consider dipolar sink that can be oriented in the direction x_1 or x_2 in the $x_1 \hat{} x_2$ plane. This attracts a mobile dipolar defect that can also be oriented in both directions. An external field interacts with the defect in orientation x_2 (with energy E_1) but not in x_1. The defect is constrained to move

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+) A drift of the point defects towards the dislocation will exist whenever in a region of attractive interaction energy there is a bias on the random walk towards the dislocation position. It means

$$\underline{J} \cdot (\underline{r}_{pd} - \underline{r}_D) < 0 \quad \text{if} \quad E_{int} (pd, D) < 0$$

linearly towards the sink and a jump from one equilibrium position to a neighbour one imposes a rotation of its symmetry axis. We also assume that when the defect is located at the saddle point configuration its interaction with other fields is null and that a x_1/x_2 oriented defect interacts (with an energy $E_2(x)$) with a x_1/x_2 oriented sink. This example is summarized in figure 3.

We will calculate the current density of defects in two cases; I: the sink is oriented in the direction x_2 parallel to the external field, II: perpendicular to it. Assuming a constant concentration of defects and an equilibrium distribution of defect orientations - Eq. (32) - it results, in case I:

$$\underline{J}^{I} = -D^{I}(E_1, E_2)\, C_0/KT\ \partial E_2/\partial x =$$

$$= -C_0\ \nu_0\ e^{-E_S/KT}\ \frac{2a}{KT}\ \hat{x}\ \frac{\partial E_2(x)}{\partial x}\ \frac{e^{-(E_1 + E_2(x))/KT}}{(e^{-(E_1 + E_2(x))/KT} + 1)^2} \qquad (34)$$

and in case II:

$$\underline{J}^{II} = -D^{II}(E_1, E_2)\, C_0/KT\ \partial E_2/\partial x =$$

$$= -C_0\ \nu_0\ e^{-E_S/KT}\ \frac{2a}{KT}\ \hat{x}\ \frac{\partial E_2(x)}{\partial x}\ \frac{e^{-E_2(x)/KT}}{(e^{-E_1/KT} + e^{-E_2(x)/KT})^2}, \qquad (35)$$

where E_S is the migration energy, "a" the distance between neighbour equilibrium positions and $\hat{x}$ the migration direction. Both E_1 and E_2 are negative. If $|E_1|$ and $|E_2|$ are smaller than KT the difference between (34) and (35) converges to zero. But it suffices one of them to be greater than KT to make the drift of dipoles towards the sink greater in case II than I. This is due to the fact in case I both the internal and external fields favour the same orientation, pinning the defect at the equilibrium site. This preferential drift is only a consequence of the anisotropy of the equilibrium configuration.

4 a) Drift of point defects towards network dislocations under a uniaxial external stress

Our aim is to determine the feasability of a dislocation climbing model

of irradiation creep. A different approach than HS and BW's one will be carried off. We shall use Eq. (30) and only first order terms for the energy - Eq. (8) - to determine if, in this approximation, the irradiation produced point defects suffer a preferential drift to different parts of the dislocation distribution when an external stress is applied. This drift, if it exists, may not give a positive contribution to the creep. Also its existence may depend only on the lattice and defects symmetry or be determined by the values of the dipole tensors at different configurations.

The diffusion equations deduced from Eq. (30) should be solved with appropriate conditions if an expression for the creep rate wanted to be obtained. This involves to consider the direction of the external applied stress with respect to the crystallographic axes, the distribution of dislocations and their full interaction with the point defects. This problem can only be tackled numerically. We shall, therefore, study the drift of point defects towards network dislocations under a particular geometry and make some approximations that allow a relatively easy solution. This approach will show some new features relevant to discuss the validity of the proposed creep mechanism. We will work in a f. c. c. lattice and consider the point defects symmetry to be determined by the dipole tensors summarized in Section 1. To be specific, the external stress will be assumed to act along a [100] direction; as this agrees with the interstitial symmetry axis relevant effects are expected . We can decompose the $\frac{1}{2}$ [110] Burgers vector of the glissile dislocations into its components parallel and perpendicular to the applied stress and consider the dominant interaction to be given by their edge components (see however Tomé and Savino, 1976). We, then, study the drift of vacancies and interstitials towards edge dislocations with their Burgers vector parallel - case I, $\hat{b}$ = [100] - or perpendicular - case II, $\hat{b}$ = [010] - to the applied stress. This entails the study of the distortion of a (001) crystallographic plane under a [100] applied stress. If those dislocations that possess a Burgers vector with a projection on the plane parallel to the stress ($\underline{b} = \frac{a}{2}$ [101]) absorb more interstitials than vacancies and, v iceversa, those with a vector that projected on the plane results perpendicular to the stress ($\underline{b} = \frac{a}{2}$ [011]) absorb more vacancies than interstitials; a deformation in the direction of the stress by dislocation climbing is obtained. Though applied to the above mentioned example the drift equations are presented in a general format.

4 b) Vacancy drift

Equation (30) is explicitly evaluated for the vacancies current density under an edge dislocation and an external uniaxial stress fields. A constant concentration C_0 of defects is assumed. In order to obtain an analytic expression, the dislocation strain field at a lattice site "j", near neighbour to "i" where the flux is evaluated, is

taken as the corresponding Taylor expansion at "i". Then, if only first order terms in this expansion are included, the change in the lattice potential energy due to the interaction between the other sources of strain and the point defect located at a position "j" near neighbour to "i", but not necessarily equivalent to it, is:

$$E_{int}^{j}\ (p.d.,\ \underline{\underline{e}}^{D} + \underline{\underline{\varepsilon}}^{ext}) = -\underline{p}^{p.d.} \cdot (\underline{\underline{e}}^{D} + \underline{\underline{\varepsilon}}^{ext})^{j} -$$

$$- \underline{\underline{p}}^{p.d} \cdot \left[(\underline{\underline{e}}^{D} + \underline{\underline{\varepsilon}}^{ext})^{i} + \underline{\underline{S}}_{ij} \cdot \nabla\, \underline{\underline{e}}^{D} \right] \qquad . (36)$$

The 12 near neighbour jumps for a vacancy in a f. c. c. lattice are introduced and the isotropic approximation is adopted for the dislocation field. An average dislocation field is considered, similary as BW did, by replacing $\frac{x_1^2}{r^2}$, $\frac{x_2^2}{r^2}$ and $\frac{(x_1\, x_2)}{r^2}$ by their mean value 1/2 whenever the dislocation strain and strain gradient fields are evaluated. This is equivalent to calculate the current of defects at positions where $|\, x_1\, | = |\, x_2\, | = \sqrt{2}\, r$, it means over directions making an angle of 45^{o} with the Burgers vector. This vector will be always taken along a x_1 direction. Within these approximation an average drift is obtained:

$$\underline{J} = C_0\, \nu_0\, a\ e^{-[E_S - \alpha(\bar{e}_{ii}^{D} + \varepsilon_{ii}^{ext})]/KT} \left\{ (\hat{x}_1 + \hat{x}_2)\, f(110, \hat{x}_1 + \hat{x}_2) \right.$$

$$\left. + (\hat{x}_1 - \hat{x}_2)\, f(1\bar{1}0, \hat{x}_1 - \hat{x}_2) + \hat{x}_1 \left[f(101, \hat{x}_1) + f(\bar{1}01, \hat{x}_1) \right] \right\} \qquad (37)$$

where

$$f(n^{VS}, \hat{x}) = \exp \left\{ \left[\underline{p}^{(n^{VS})} \cdot (\underline{\bar{e}}^{D} + \underline{\underline{\varepsilon}}^{ext}) \right] / KT \right\}$$

$$\left\{ 2 \sinh \left[\hat{x} \cdot \bar{\nabla} \left(2\alpha\, \underline{\underline{I}} - \underline{p}^{(n^{VS})} \right) \cdot \underline{\underline{e}}^{D} / 2\, KT \right] - \right.$$

$$\left. - 2 \sinh \left[\hat{x} \cdot \bar{\nabla} \left(-\underline{p}^{(n^{VS})} \right) \cdot \underline{\underline{e}}^{D} / 2\, KT \right] \right\}$$

$\bar{e}$, $\bar{\nabla}$ means average strain and gradient field in the above defined sense and use has been of the fact that $\bar{\nabla}_{x_2} (\underline{\underline{e}}_{11}^{D} + \underline{\underline{e}}_{22}^{D}) = 0$ - were not for this relation another term in the direction x_2 would have appeared in Eq. (37). 2 a is the lattice parameter, E_S the vacancy migration energy in a strain free

body and Eq. (14) has been used.

We consider the applied stress parallel to the dislocation Burgers vector (case I) and perpendicular to it (case II). The difference in vacancies drift between cases I and II results - using Eqs. (15), (20), (21) and (37) - :

$$\underline{\bar{J}}^{II} - \underline{\bar{J}}^{I} = C_0 \; \nu_0 \; a \; \hat{x}_1 \; e^{-\left\{ E_S - \alpha \left[\bar{e}_{ii}^{D} + (1-2\nu)\varepsilon \right] \right\}/KT}$$

$$\exp\left\{ (g_1 \; \bar{e}_{11}^{D} + g_3 \; \bar{e}_{22}^{D})/KT \right\} \left\{ \left\{ 4 \sinh \left\{ \bar{\nabla}_{x_1} \left[(-g_1 + 2\alpha) e_{11}^{D} + (-g_3 + 2\alpha) \; e_{22}^{D} \right] \right. \right. \right.$$

$$\left. \left. \left. /2 \; KT \right\} - 4 \sinh \left[\bar{\nabla}_{x_1} (-g_1 \; e_{11}^{D} - g_3 \; e_{22}^{D})/2 \; KT \right] \right\} \right\}$$

$$\left\{ \exp (g_3 - 2\nu \; g_1) \; \varepsilon \; /KT - \exp \left[-\nu \; (g_3 + g_1) + g_1 \right] \varepsilon \; /KT \right\} \quad (38).$$

As the defect symmetry in a f. c. c. lattice imposes g_3 to be bigger than g_1, we conclude from Eq. (38) that more vacancies drift towards the edge dislocation in case II than I. This conclusion agrees with the one obtained by BW and supports HS's mechanism. It is based, however, on a completly different approach to the problem. The reason for this preferential drift resides in the symmetry of the saddle point configuration.

4 c) Interstitial drift

The interstitial case is more complex than the vacancy one. The dumbbell interstitial may adopt three orientations at a given site. As discussed in Section I, these are not equivalent when another source of internal stress is present. In the diffusion equations the fact must be included that the migration of the interstitial to a nearest neighbour position results in a rotation of its symmetry axis. We assume a constant interstitials concentration ($C_i = C_0$) and that the distribution of the defect orientations at a given site is given by the equilibrium distribution - Eq. (32) -. With the same assumptions that in the vacancy case, the average drift of interstitials towards a dislocation under an external stress results:

$$\underline{\bar{J}} = 4 \; C_0 \; \nu_0 \; a \; e^{-E_S/KT} \left[\underline{\underline{p}}_K^{(100)} \cdot (\underline{\underline{\bar{e}}}^{D} + \underline{\underline{\varepsilon}}^{ext}) + \underline{\underline{p}}_K^{(010)} \cdot (\underline{\underline{\bar{e}}}^{D} + \underline{\underline{\varepsilon}}^{ext}) \right.$$

$$\left. + \underline{\underline{p}}_K^{(001)} \cdot (\underline{\underline{\bar{e}}}^{D} + \underline{\underline{\varepsilon}}^{ext}) \right]^{-2} \left\| \hat{x}_1 \left\{ F \left[\begin{pmatrix} 100 \\ 110 \end{pmatrix}, \; x_1 \; , \; x_2 \right] \right. \right.$$

$$+ F\left[\binom{010}{110}, x_1, x_2\right] + F\left[\binom{100}{101}, x_1, 0\right] +$$

$$F\left[\binom{001}{101}, x_1, 0\right]\Big\} + \hat{x}_2 \Big\{ F\left[\binom{100}{110}, x_2, x_1\right] + F\left[\binom{010}{110}, x_2, x_1\right]$$

$$+ F\left[\binom{010}{011}, x_2, 0\right] + F\left[\binom{001}{011}, x_2, 0\right] \Big\}\Big\| \qquad (39)$$

where

$$F\left[\binom{n}{n_{ij}}, x, y\right] = \exp\left[\underline{\underline{p}}_K \binom{n}{n_{ij}} \cdot \left(\underline{\underline{e}}^D + \underline{\underline{\varepsilon}}^{ext}\right)\right]$$

$$\left[f_x \cosh_x \binom{n}{n_{ij}} \cosh_y \binom{n}{n_{ij}} + f_y \sinh_x \binom{n}{n_{ij}} \sinh_y \binom{n}{n_{ij}}\right]$$

$$\sinh/\cosh_{x,y} \binom{n}{n_{ij}} = \sinh/\cosh\left(\frac{\underline{p}_K \binom{n}{n_{ij}}}{2} \frac{\bar{\partial}}{\partial x, y} \underline{\underline{e}}^D\right)$$

$$\sinh/\cosh_0 \binom{n}{n_{ij}} = 0/1$$

$$\underline{\underline{p}}_K = \underline{\underline{p}}/KT$$

and

$$f_{x,y} = \sum_{n=\begin{cases}100\\010\\001\end{cases}} e^{\underline{p}_K^{(n)}} \left(\underline{\underline{e}}^{-D} + \underline{\underline{\varepsilon}}^{ext}\right) \underline{\underline{p}}_K^{(n)} \cdot \frac{\bar{\partial}}{\partial x, y} \underline{\underline{e}}^D$$

We want to compare Eq. (39) in cases I and II previously defined. This is more difficult than in the vacancy case due to the anisotropy of both the equilibrium and saddle point configurations. In the example of Section 3 b) we found that he anisotropy of the equilibrium configuration imposes a different drift in the two cases considered. In the present case, as the external stress is assumed to be small, the expansion:

$$e^{\bar{E}/KT} = \left[\sum_n e^{\underline{p}_K^{(n)}} \cdot \left(\underline{\underline{e}}^{-D} + \underline{\underline{\varepsilon}}^{ext}\right)\right]^{-1} \simeq$$

$$\simeq \left[\sum_n \underline{\underline{e}}^{\underline{p}_K^{(n)}} \cdot \underline{\underline{e}}^{-D} \left(1 + \underline{p}_K^{(n)} \cdot \underline{\underline{\varepsilon}}^{ext}\right)\right]^{-1} \qquad (40),$$

where $\bar{E}$ has been defined in Eq. (34), is allowed. Assuming the interstitial as a strong defect (high value of $\underline{\underline{p}}$), what seems to be the case in Cu -Table I-, relatively strongly anisotropic ($\lambda_2 \geq 1.1\ \lambda_1$, assumption not completly fulfilled by some of the values in Table I) and its symmetry at equilibrium given by Eq. (16) and using Eq. (28); Eq. (40) approaches to the value:

$$e^{\bar{E}/KT} \simeq e^{-\underline{\underline{p}}_K^{(010)} \cdot \underline{\underline{e}}^D} \left(1 + \underline{\underline{p}}_K^{(010)} \cdot \underline{\underline{\xi}}^{ext}\right)^{-1} \quad (41).$$

Approximation that can be numerically justified. Comparing equation (41) in cases I and II by using Eqs. (16), (20) and (21), it results:

$$e^{\bar{E}^I/KT} < e^{\bar{E}^{II}/KT} \quad (42)$$

If the saddle point configuration were spherically symmetric, the relation (42) would mean that the amplitude of the interstitial drift towards the dislocation is greater in case II than I. The reasons for this difference in drift are equivalent to those discussed in the example of Section 3 b). We conclude, that, if the approximation of a spherically symmetric saddle point configuration and those leading to Eqs. (39) and (42) hold, a creep process in the direction of the applied stress would not be sustained by interstitials stress assisted diffusion.

We continue the analysis of Eq. (39) with the above assumptions about the equilibrium configuration but considering the saddle point symmetry to be given by Eq. (17). If the dipole tensor at this configuration is assumed strongly anisotropic the relevant interaction with the dislocation would correspond to a jump from a (010) / (001) orientation towards a (011) neighbour. This means we expect a strong difference between the average drift in cases I and II in the x_2 direction. We, then, find this difference proportional to:

$$|\bar{J}^I| - |\bar{J}^{II}| \propto \left(\underline{\underline{p}}_K^{\binom{010}{011}} - \underline{\underline{p}}_K^{(010)}\right) \cdot \left(\underline{\underline{\xi}}^{ext^I} - \underline{\underline{\xi}}^{ext^{II}}\right). \quad (43)$$

Using Eqs. (16), (17), (20) and (21) we conclude:

$$|\bar{J}^I| \begin{matrix} > \\ \text{or} \\ < \end{matrix} |\bar{J}^{II}| \quad \text{if} \quad (g_3 - \lambda_2) \begin{matrix} > \\ \text{or} \\ < \end{matrix} (g_1 - \lambda_1) . \quad (44)$$

This simple relation only holds under the previous approximations, but it shows that the feasability of the proposed preferential drift depends on the values of the dipole tensor at the interstitial saddle point and equilibrium configuration.

5. Discussion

Though calculations of defects configuration have achieved a high sophistication, an analytic framework did not exist either to calculate their interaction with an external stress, until the recent work of Dederichs et al. (1975), or with internal sources of distorsion. Continuum approximations are therefore generally applied to calculate the interaction energy between internal centers of distortion in the crystal. In the case of point defects this approach implies to use a set of parameters related "ad hoc" with more accurate calculations of the defect configuration. In Section 2 of this work a general equation - Eq. (8) - was deduced to calculate the interaction energy between a point defect and a source of internal stress, including the discrete nature and anisotropy of the defect. This equation together with the "soft point defect approximation" is used to calculate the interaction energy between a vacancy and an edge dislocation in a strained copper crystal. The approximation of considering the point defect to be "soft" entails to include in the calculation only anharmonic terms in the interaction between the defect and the host atoms in an otherwise harmonic lattice. This agrees with Tewary's Green's function approach (1973) to calculate the defect configuration. Consistently Tewary's model for the vacancy (1969) is used. The amplitude of the interaction energy results bigger when the stress is applied perpendicular to the Burgers vector of the dislocation than in the case of a perpendicular stress. This preference agrees with BW's results. When the interaction energy between a dumbbell interstitial in a strained f. c. c. crystal and an edge dislocation is calculated, both the anisotropy of the defect dipole tensor and the stress induced interaction are relevant. The interaction depends on the orientation of the interstitial with respect to the dislocation. The soft point defect approximation results too crude for the interstitial case. If the stress induced interaction with a dislocation wanted to be evaluated, a computer simulation of the interstitial configuration is presence of the dislocation and external strain field should be performed. However, as discussed in Section 2, either using Dederichs et al. results (1975) or accepting the soft point defect approximation we found the external stress to enhance preferentially the interaction between the interstitial and the dislocation with Burgers vector perpendicular to the applied stress. This result contradicts BW's one.

In Section 3 and 4 we discuss the drift of point defects towards edge dislocations in a strained crystal. When anisotropic point defects are considered and the lattice symmetry introduced the continuum equations for the flux of point defects in a stress field must be replaced by one that considers the discrete character or the jump and the defect equilibrium and saddle point configurations. The equation proposed by Kronmüller et al. (1971) for the defects current

density is used in the work. It is argued that a preferential drift towards different parts of the dislocation distribution may exist in a strained crystal due to the anisotropy of the defect configuration. To prove this, the stress induced dislocation point defect interaction discussed by BW and by us in Section 2 is not included in the calculation. The drift is discussed towards edge dislocations with the Burgers vector parallel and perpendicular to the external stress. A mean isotropic strain field is introduced for the dislocation in agreement with BW's suggestion. This implies to consider the average drift towards the dislocation to be given by the defects current density on points located at 45° with the Burgers vector and in a plane perpendicular to the dislocation line. The dislocation strain and the external stress modifies the local diffusivity. This influences the net drift towards one orientation or the other of the dislocation distribution. The relative importance of this effect with respect to the stress induced interaction discussed by BW depends on the degree of anisotropy of the defect equilibrium and saddle point configurations, and requires further numerical calculations to be asserted.

The example discussed in the text shows that the drift of vacancies is favoured in a f. c. c. lattice towards edge dislocations with their Burgers vector perpendicular to the applied stress. This result is in agreement with HS's model of creep by dislocation climbing, but the effect studied by us is due to the symmetry of the vacancy saddle point configuration. For the dumbbell interstitial in copper, both equilibrium and saddle point configurations, according to the results reported in Table I, have a comparable degree of anisotropy. This may determine the stress induced interaction to become more relevant than the drift term studied by us. We found the trend in HS' mechanism of creep would be also favoured by the drift of the dumbbell interstitial in a f. c. c. lattice if the saddle point configuration were more anisotropic (larger relative difference between the dipole tensor eigenvalues) than the equilibrium one. The main conclusion is that the proposed mechanism of creep can be only sustained if some relations are fulfilled by the equilibrium and saddle point configurations of the migrating defects.

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Table I

Dipole tensor for a vacancy and a dumbell interstitial in copper

Defect configuration	Approximation	Interatomic potential	p_1 [eV]	p_2 [eV]	p_3 [eV]	References
(1oo) Dumbell Interstitial	Kanzaki forces	Morse[a]	[1oo] 21.36	[o1o] 22.53	[oo1] 22.53	Dederichs (1975), Schober and Dederichs
		Born Mayer[b]	[1oo] 12.7	[o1o] 13.2	[oo1] 13.2	Schober and Dederichs
	Soft point defect	Born Mayer[c]	[1oo] 4.47	[o1o] 11.69	[oo1] 11.69	Tewary (1969)
Vacancy	Kanzaki forces	Morse[a]	[1oo] -.15	[o1o] -.15	[oo1] -.15	Schober and Dederichs
	Soft point defect	Born Mayer[c]	[1oo] -3.43	[o1o] -3.43	[oo1] -3.43	Tewary (1969)
(1oo, 11o) Dumbell interstitial saddle point	Kanzaki forces	Morse[a]	$[11o]/\sqrt{2}$ 25.o	$[1\bar{1}o]/\sqrt{2}$ 19.7	[oo1] 23.3	Dederichs (1975) Schober and Dederichs
		Born Mayer[b]	$[11o]/\sqrt{2}$ 14.4	$[1\bar{1}o]/\sqrt{2}$ 11.6	[oo1] 13.5	Schober and Dederichs
	Soft point defect	Born Mayer[c]	$[11o]/\sqrt{2}$ 5.98	$[1\bar{1}o]/\sqrt{2}$ 4.7o	[oo1] 5.51	Johnson[d]
ooo → 11o Vacancy saddle point	Soft point defect	Born Mayer[c]	$[11o]/\sqrt{2}$ -4.76	$[1\bar{1}o]/\sqrt{2}$ -.49	[oo1] -1.16	Johnson[d]
	Kanzaki forces	Morse[a]	$[11o]/\sqrt{2}$ -.4	$[1\bar{1}o]/\sqrt{2}$ 1.4	[oo1] 6.6	Schober and Dederichs

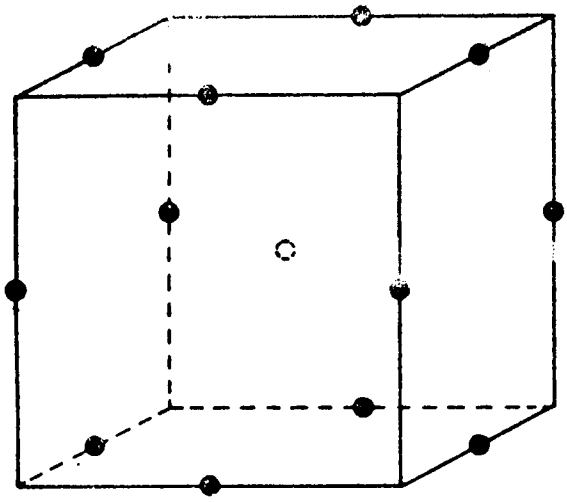
(a) Doyama and Cotterill (1965)

(b) Gibson, Goland, Milgram and Vineyard (196o)

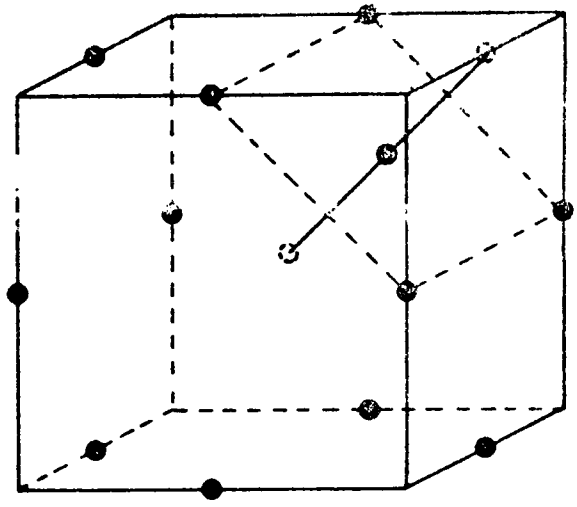
(c) Huntington and Seitz (1942), Huntington (1953)

(d) Girifalco and Welch (1967) .

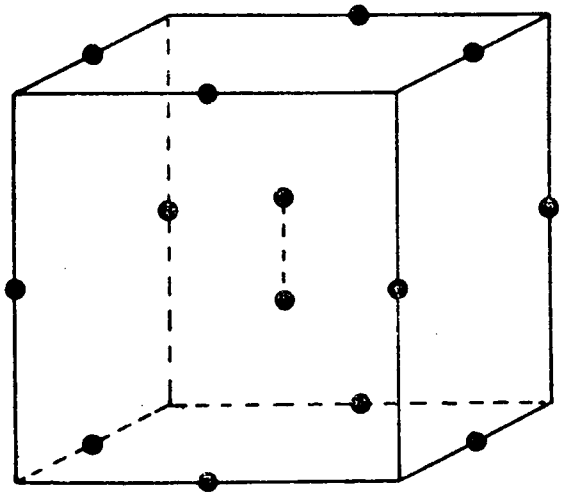
Figure 1



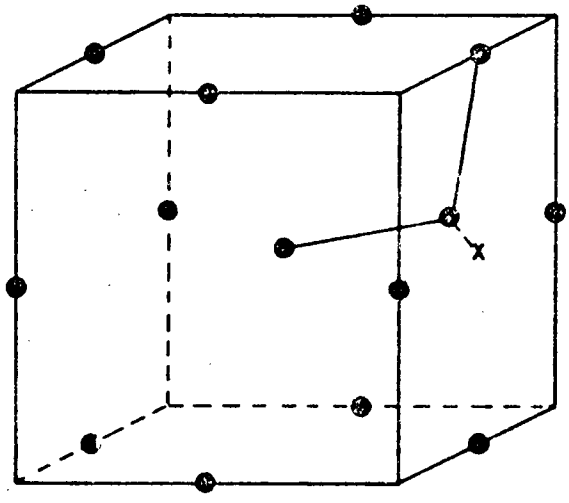
1 a - Vacancy equilibrium configuration



1 b - Vacancy saddle point configuration



1 c - (1oo) dumbbell interstitial configuration



1 d - Dumbbell interstitial saddle point

Figure 2

Figure 3