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Drift Diffusion of Radiation-produced Point Defects to Edge Dislocation

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Abstract

Under the heavy irradiation, when the production and the recombination of interstitials and vacancies are included, the diffusion equations become nonlinear. An effort has been made to arrange an appropriated transformation of these nonlinear differential equations to soluble Poisson's equations, so that analytical solutions for simultaneously calculating the concentrations of interstitials and vacancies in the angular dependent Cottrell's potential of the edge dislocation have been derived from the well-known Green's theorem and perturbation theory.

1. Introduction

When the solid material is irradiated by the energetic particles, the equal numbers of the interstitials and vacancies (hereafter denoted by i and v) are produced in the matrix. As the concentration of i and v increase, they will be recombined significantly by each other as well as absorbed by the sinks such as grain boundaries, dislocations, external surfaces, etc.

It is particularly known that the dislocation absorbs i more preferentially than v, so that the excess of v will be built up in a certain region of matrix. Such an idea leads one to believe that the dislocation plays an important role on the nucleation of voids and irradiation-enhanced creep of materials during the heavy irradiation

In order to figure out the possibility of such phenomena, one should solve the appropriate diffusion equations with an assumption that such phenomena are associated with diffusion of i and v under the conditions mentioned above.[1-5] In doing so, one will encounter a couple of difficulties: First, when the production and recombination of i and v are included, the diffusion equations become nonlinear. Second, the interaction potential (e.g. the Cottrell's potential) of the edge dislocation is angular dependent. Those problems are troublesome so that some works in the field have omitted all or some of them[6-9]. In fact, both should be included for these nonlinear differential equations to be solved as seen in the following sections. While some other did included them but calculated the results numerically[10-11]. Since the production and recombination of i and v are very important physical processes, the omission of them can result in serious errors in

understanding and interpreting the observations

This paper presents an analytical solution for calculating the concentrations of i and v simultaneously in angular dependent Cottrel's potential field of the edge dislocation during heavy irradiation by means of the well-known Green theorem and the perturbation theory. The transformation of nonlinear diffusion equations to the soluble equation and applicability of perturbation theory will be examined in Sec. 2. The boundary conditions and the Green theorem will be discussed in Sec. 3.

2. Diffusion Equations and Their Transformation to Soluble Equations

2.1 Nonlinear Diffusion Equations

When the recombination of i and v becomes significant, the concentrations of i and v should satisfy

$$\partial C_i / \partial t = -\nabla \cdot \mathbf{J}_i + \dot{n} - R_{iv} C_i C_v \qquad (1a)$$

$$\partial C_v / \partial t = -\nabla \cdot \mathbf{J}_v + \dot{n} - R_{iv} C_i C_v \qquad (1b)$$

where $\dot{n}$ is the production rate of i and v by the irradiation, R_{iv} is the recombination rate of i and v, and C_α is the concentration of the α-type defect (α denotes i or v). In Eq.(1a) and (1b), the thermal generation of i and v was neglected in compared with $\dot{n}$.

Substitution of the current density[12],

$$\mathbf{J}_\alpha = -D_\alpha \left(\nabla C_\alpha + \beta C_\alpha \nabla \phi_\alpha \right), \qquad (2)$$

in the cottrell's potential of the edge dislocation ϕ_α, where

$$\phi_\alpha = K_\alpha (\cos\theta / r) \qquad (3)$$

with

$$K_\alpha = \left(\frac{\mu b}{3\pi} \frac{1+\nu}{1-\nu} \right) \Omega_0 \Delta a_\alpha , \qquad (4)$$

for Eq.(1a) and (1b) gives, at the quasi-steady state conditions,

$$D_i \left(\nabla^2 C_i + \beta C_i \nabla \phi_i \right) + \dot{n} - R_{iv} C_i C_v = 0 \qquad (5a)$$

$$D_v \left(\nabla^2 C_v + \beta C_v \nabla \phi_v \right) + \dot{n} - R_{iv} C_i C_v = 0 \qquad (5b)$$

where D_α is the diffusion coefficient of α-type defects; $k_B T = 1/\beta$ is the usual meaning of thermal energy; μ, b, ν, Ω_0, and Δa_α are the shear modulus, the Burgers vector, the Poisson's ratio, the atomic volume, and the dilation (in unit of Ω_0) due to the α-type defect respectively; and $\mathbf{r}(r, \theta)$ is the polar coordinate of the defect with respect to the edge dislocation with the angle θ measured from its extra plane. In these Eq. (5a) and (5b), we neglected the dislocation movement due to absorption of i and v.

2.2 Transformation to Soluble Equations

For simplicity, taking

$$R = R_{iv} / \left(D_i D_v\right), \tag{6}$$

$$DC = (\dot{n} / R)^{\frac{1}{2}} (1 - S), \tag{7}$$

$$\alpha_0 = (\dot{n} R)^{\frac{1}{4}}, \tag{8}$$

and

$$z = \alpha_0 r, \tag{9}$$

then

$$(\nabla^2 - 1) S_i = -\beta \nabla S_i \cdot \nabla \phi_i + S_v (1 - S_i) \tag{10a}$$

$$(\nabla^2 - 1) S_v = -\beta \nabla S_v \cdot \nabla \phi_v + S_i (1 - S_v) \tag{10b}$$

It will be discussed in Sec.3.3. that the right-hand sides of Eq. (10a) and (10b) are small enough to be treated as the perturbation.

The differential equation,

$$\left(\nabla^2 - 1\right) S = 0, \tag{11}$$

does not look like Laplace equation. However, since $S(\mathbf{z})$ is axially independent, the equation is adjustable to be the modified Bessel function.

3.0 Analytical Solutions

3.1 Boundary Conditions

Generally speaking, the defects would jump by a distance d (the jumping distance) per a jump. However, as the closer they approach to the dislocation, the larger the elastic interaction becomes. When they reach at a certain distance, they would jump directly to the center through the rapid rearrangement of lattice atoms near the dislocation core. It is referred to as the "core radius". which is the inner boundary. In such a case, the migration energy of the defects inside the core radius is smaller than the thermal energy as shown in Fig. 1. It is therefore true that the core radius is dependent upon the various parameters including the temperature, the interaction strength, etc.

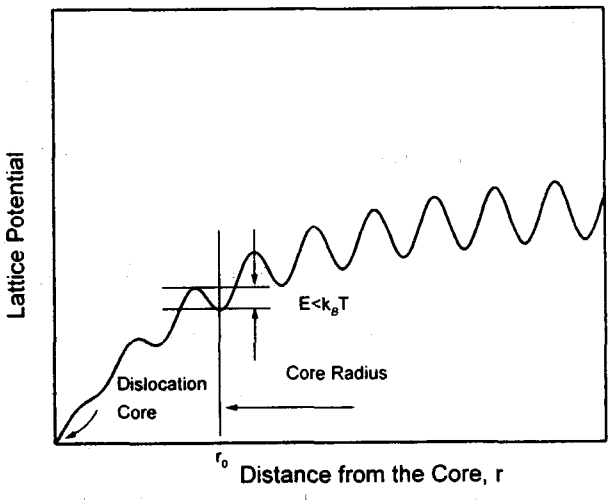

Fig.1. Lattice Potential Near the Dislocation Core

From the reason mentioned above, the boundary condition on the inner surface (r_0 : the core radius) can be naturally

$$C_\alpha(r_0) = 0 \quad \text{or} \quad S_\alpha(r_0) = 1 \tag{12}$$

On the other hand, the condition on the outer boundary surface (r_b : the mid-point between dislocations) is

$$\left.\partial C_\alpha / \partial r\right|_{r=r_b} = 0 \quad \text{or} \quad \left.\partial S_\alpha / \partial r\right|_{r=r_b} = 0 \tag{13}$$

which is true only when the perturbations (right-hand sides of Eq. (10)) are not taken into account. However, when the interaction between the dislocation and point defects is considered, there are some amount of flow-in and flow-out of i and v (referred to as "drift diffusion") through the outer boundary surface.

3.2 Analytical Solutions

In order to apply Green theorem and perturbation theory, we expend $S_i(\mathbf{z})$ and $S_v(\mathbf{z})$ in the space where $cos\theta$ is one of the eigen-functions, that is,

$$S_i(\mathbf{z}) = \sum_{n=-\infty}^{+\infty} F_n(z) e^{in\theta}$$

$$= F_0(z) + 2\sum_{n=1}^{+\infty} F_n(z)\cos n\theta \tag{14a}$$

and

$$S_v(\mathbf{z}) = H_0(z) + 2\sum_{n=1}^{+\infty} H_n(z)\cos n\theta . \tag{14b}$$

Then the differential equation for i {Eq.(10a)} becomes

$$\left[\frac{\partial^2}{\partial z^2} + \frac{1}{z}\frac{\partial}{\partial z} - \left(1 + \frac{n^2}{z^2}\right)\right] F_n(z) = -4\pi\rho_n(z) \tag{15}$$

where

$$\rho_n(z) = \rho_n^d(z) + \rho_n^r(z) \tag{16}$$

with

$$\rho_n^d(z) = -\frac{\alpha_0 \beta K_i}{8\pi z^2}\left(F_{n-1}' + \frac{(n-1)}{z}F_{n-1} + F_{n+1}' - \frac{(n+1)}{z}F_{n+1}\right), \tag{17}$$

$$\rho_0^r(z) = -\frac{1}{4\pi}\left[H_0(1 - F_0) - 2\sum_{m=1}^{\infty} F_m H_m\right], \tag{18a}$$

and

$$\rho_n^r(z) = -\frac{1}{4\pi}\left(H_n - \sum_{m=0}^{\infty} F_m H_{n+m} + F_{n+m} H_m\right) \text{ for } n \geq 1 . \tag{18b}$$

In Eq.(17), the prime denotes the derivative with respect to z.

The solutions are

$$F_n(z) = \psi_n(z) + f_n^d(z) + f_n^r(z) \qquad (19)$$

where $\psi_n(z)$ are the general solutions of

$$\left[\frac{\partial^2}{\partial z^2} + \frac{1}{z}\frac{\partial}{\partial z} - \left(1 + \frac{n^2}{z^2}\right)\right]\psi_n(z) = 0 \quad (20)$$

which is the modified Bessel function, $f_n^d(z)$ are the special functions due to the drift diffusion associated with $\rho_n^d(z)$, and $f_n^r(z)$ are that (refer to as recombination) related with $\rho_n^r(z)$. We have the corresponding solutions for v as

$$H_n(z) = \psi_n(z) + h_n^d(z) + h_n^r(z). \qquad (21)$$

Among $\psi_n(z)$, only one that satisfied the boundary conditions (Eqs. (12) and (13)) is

$$\psi_0(z) = \frac{K_1(z_b)I_0(z) + I_1(z_b)K_0(z)}{K_1(z_b)I_0(z_0) + I_1(z_b)K_0(z_0)} \quad (22)$$

and others, which do not satisfy, are

$$\psi_n(z) = 0 \quad \text{for } n \geq 1.$$

Having the Green function of

$$G(\mathbf{z},\mathbf{z}') = \sum_{n=-\infty}^{+\infty} g_n(z,z')e^{in(\theta-\theta')} \qquad (23)$$

with

$$g_n(z,z') = A_n\left[I_n(z_0)K_n(z_<) - K_n(z_0)I_n(z_<)\right] \times \left[I_n(z_b)K_n(z_>) - K_n(z_b)I_n(z_>)\right] \qquad (24)$$

and

$$A_n = 2/\left[I_n(z_0)K_n(z_b) - K_n(z_0)I_n(z_b)\right]$$

where $z_>$ ($z_<$) is the larger (smaller) of z and z', as we usually do, the special solutions are given by

$$f_n^d(z) = \int g_n(z,z')\rho_n^d(z')z'dz' \qquad (25a)$$

and

$$f_n^r(z) = \int g_n(z,z')\rho_n^r(z')z'dz'. \qquad (25b)$$

So that, from Eq.(19), we conclude

$$F_0(z) = \psi_0(z) + f_0^d(z) + f_0^r(z) \qquad (26a)$$

$$F_n(z) = f_n^d(z) + f_n^r(z) \quad \text{for } n \geq 1. \quad (26b)$$

$H_n(z)$ for v can be easily obtained by exchanging the interaction strength K_i in $\rho_n^d(z)$ (Eq. (17)) for K_v. As the results, $H_n(z)$ have also been done as soon as $F_n(z)$ have been calculated.

3.3 Perturbations

The first term (drift term) in the right- hand side of Eq. (10) is small in the region under consideration since the region, where the interaction field is large, is excluded by the dislocation core. The second term (recombination term) is also small since $S \leq 1$ and $(1-S) \leq 1$, so that the value of $S(1-S)$ is smaller than the smaller of S and $(1-S)$. As the results, the maximum value of $S(1-S)$ is 0.25 as shown in Fig. 2 since S is almost equal to ψ_0.

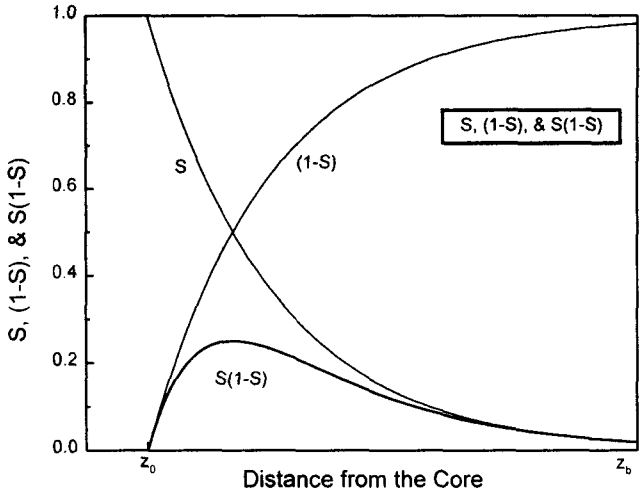

Fig.2. Value of S, (1-S), and S(1-S)

4. Conclusions

Since drift term (interaction term) and recombination term are small enough for $S(z)$ to be $\psi_0(z)$ at the zero order approximation, which is the case of Eq. (11), $f_0^d(z)$ and $f_0^r(z)$ are calculated through Eq. (25a) and (25b). If $f_0^d(z)$ and $f_0^r(z)$ are small sufficiently (they are expected to be so), $f_n^d(z)$ and $f_n^r(z)$ all for $n \geq 1$ can be evaluated with $\psi_0(z)$ only until they converge.

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