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Diffusion under a stress in fcc and bcc metals

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Abstract

This work is devoted to the evaluation of a change in the barrier height in the case of an atom jump to the nearest vacancy site under strain and to obtaining the vacancy diffusion equation taking into consideration the strain influence. Earlier, we suggested a new approach to solving the problem of the influence of elastic stress on the vacancy jump rate for atomic diffusion in crystals. It was based on the simple observation that a stress field alters the surrounding configuration and on the assumption that the height of the activation barrier should be altered accordingly. The change of the activation barrier was shown to depend on the displacement field, the symmetry of the crystal, the atomic structure near point defects and the interatomic potential. Knowledge of this change makes it possible to calculate the jump rate. The expression for the vacancy flux was obtained with the help of the ‘hole gas’ method, by using the jump rate. In these nonlinear equations, the influence of the strain tensor component on diffusion flux is determined by coefficients, which depend on the atomic interaction and atomic structure of the saddle-point configuration. One of the aims of the present work is to generalize our approach taking into account N-body interatomic interaction. Now we present the diffusion equation for vacancy in FCC and BCC metals, obtained in a more general and convenient form.

1. Introduction

Elastic fields, generated by defects of the structure, influence the diffusion process. In addition, as a result, it leads to the alteration of the phase transformation kinetic, segregation formation and changes in the system properties. However, understanding the effects of pressure and strain on diffusion in solids is now limited. Usually, the equation of diffusion in the presence of stress field has the following form [1]:

$$\mathbf{J}_F = -D \left(\nabla c + c \frac{\nabla U}{k_B T} \right), \quad (1)$$

where \mathbf{J}_F is the flux of impurity atoms or defects, c is the concentration of impurity atoms or defects, D is the corresponding diffusion coefficient under zero strain, k_B is Boltzmann’s constant, T is the temperature, U is an interaction potential of the diffusing atoms with the defects generating stress fields. Some authors consider point defects as the centers of dilatation [2]. Equation (1) is similar to one, describing

the electric field influence on the diffusion flux. At the same time, this expression does not take into account the principal difference between the effect of electrical field, which directly affects a jumping atom and the elastic field, the influence of which is realized through the neighbors surrounding this atom. It is clear, that for the second case the effect must depend on the geometry of the arrangement of neighboring atoms and, consequently, on crystallographic structure.

Equation (1) is too crude for objects of atomic size. This one and some other approximations [3] do not take into account the atomic structure in the neighborhood of the defect and stresses, which essentially influence the energy of a jumping atom [3, 4]. Furthermore, very few papers have considered, that shear stress can modify the atomic jump frequency [4–6]. There are some earlier works devoted to the effects of elastic strain on energetic contributions to the free energy barrier to diffusional motion [5–8], as well as describing elastic strain effects on the contribution to the migration barrier of interaction of the migrating defects with conduction electrons and on the contribution to the lattice-vibrational entropic [8].

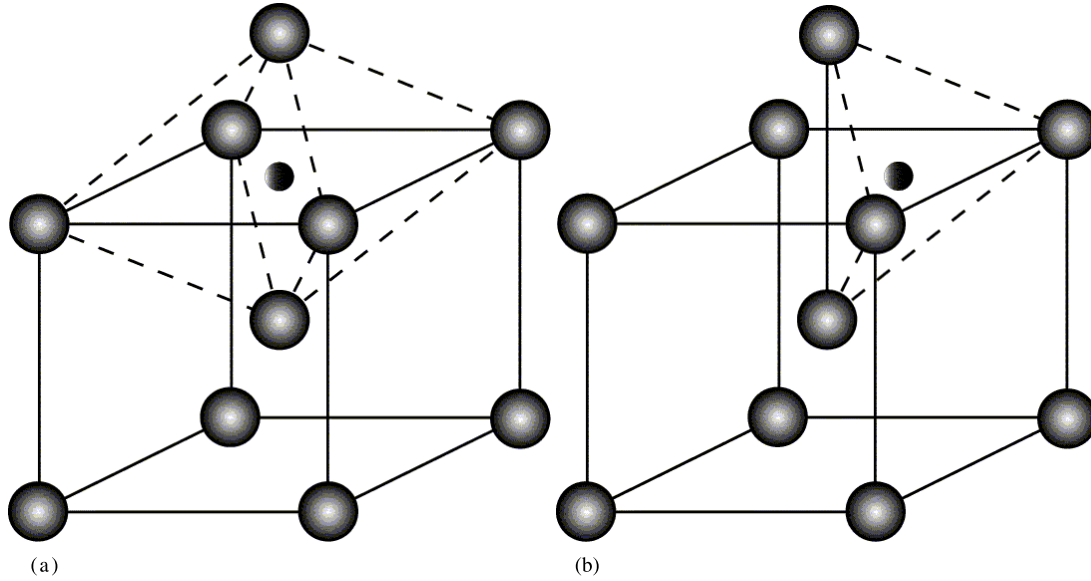


Figure 1. Positions of interstitial atom in the bcc structure. (a) Equilibrium configuration, (b) saddle-point configuration.

The importance of the anisotropy of the saddle point was first pointed out by Koehler [5].

Let us consider, for example, an interstitial atom in bcc lattice (figure 1) to illustrate the features of our approach. The interstitial atom energy depends on the distance between this atom s and its neighboring atoms: $E_s = E(\mathbf{r}_1 - \mathbf{r}_s, \dots, \mathbf{r}_k - \mathbf{r}_s, \dots)$, $k \in \{1, \dots, n\}$, where n is the number of atoms in the system.

The displacement field changes the distances between interstitial atom and metal atoms and, consequently, interstitial atom energy. $E_s = E_s(\mathbf{r}_k + \mathbf{u}_k - \mathbf{r}_s - \mathbf{u}_s)$. Here $\mathbf{u}_k \equiv \mathbf{u}(\mathbf{r}_k)$ is the displacement of atom k , which is a function of its location \mathbf{r}_k . This is true both for the equilibrium configuration (figure 1(a)) and for the saddle-point configuration (figure 1(b)) and it is the starting point of our approach [9–12]. As the stress fields can alter the atomic configuration of the defect environments, the local magnitude of the activation barrier for defect transition in different directions is altered in accordance with the configuration change. Knowing this alteration, we calculated the atomic jump rates and obtained equations for the fluxes in interstitial alloys with fcc and bcc structures [13].

In a similar way we obtained early equations for the fluxes of the vacancies in fcc [9, 11] and bcc [10] metals. In this paper, we continue the investigation of diffusion under strain, generalize our approach and apply it to study the stress influence on diffusion vacancy in these metals. We present the diffusion equation for vacancy, obtained for a general case and in another more convenient form. In particular, one of the aims of the present work is to generalize our approach taking into account the possibility of N-body interatomic interaction.

2. Main moments of theory of diffusion under a stress

We consider vacancy diffusion in cubic crystals in the presence of a stress field. As pointed out above, the equilibrium positions of atoms are changed due to the displacement field and the potential energy of atoms is changed accordingly. This

is true whatever the position of the atom under consideration, in saddle as well as in an equilibrium configuration. As shown in [12] the change of the atom energy under strain is given by the following equation:

$$\Delta E_s = \sum_k \frac{1}{R_{ks}} \frac{\partial E_s}{\partial R_{ks}} (x_{ks}^2 \varepsilon_{11} + y_{ks}^2 \varepsilon_{22} + z_{ks}^2 \varepsilon_{33} + 2x_{ks} y_{ks} \varepsilon_{12} + 2x_{ks} z_{ks} \varepsilon_{13} + 2y_{ks} z_{ks} \varepsilon_{23}), \quad (2)$$

where x_k, y_k, z_k are the coordinates of the atom k , $x_{ks} = x_k - x_s, y_{ks} = y_k - y_s, z_{ks} = z_k - z_s, k \neq s, R_{ks} = |\mathbf{r}_k - \mathbf{r}_s| = \sqrt{x_{ks}^2 + y_{ks}^2 + z_{ks}^2}$ for all atoms k , and $\varepsilon_{ij} = (1/2)(\partial u_i / \partial x_j + \partial u_j / \partial x_i)$ is the strain tensor ($i, j = 1, 2, 3$).

Now it is necessary to evaluate the change of a system energy E that in the case of N-body potentials can be written as [14]

$$E = \sum_s f(\rho_s) + \frac{1}{2} \sum_s \sum_k \Phi(\mathbf{r}_{sk}), \quad \rho_s = \sum_{k \neq s} \varphi(\mathbf{r}_{sk}), \quad (3)$$

where Φ and f are functions describing N-body potential, ρ_s is electron density in the point of atom s position, φ is a function determining a contribution of each atom in electron density. If the system energy $E = E(x_k - x_s, y_k - y_s, z_k - z_s), (k = 1, 2, \dots, n)$, then the change of the system energy conditioned by strain is

$$\Delta E = \sum_s \left[\sum_{k \neq s} \left(\frac{x_{ks}^2}{R_{ks}} \frac{\partial E}{\partial R_{ks}} \right) \varepsilon_{11}(\mathbf{r}_s) + \sum_k \left(\frac{y_{ks}^2}{R_{ks}} \frac{\partial E}{\partial R_{ks}} \right) \varepsilon_{22}(\mathbf{r}_s) + \sum_k \left(\frac{z_{ks}^2}{R_{ks}} \frac{\partial E}{\partial R_{ks}} \right) \varepsilon_{33}(\mathbf{r}_s) + 2 \sum_k \left(\frac{x_{ks} y_{ks}}{R_{ks}} \frac{\partial E}{\partial R_{ks}} \right) \varepsilon_{12}(\mathbf{r}_s) + 2 \sum_k \left(\frac{x_{ks} z_{ks}}{R_{ks}} \frac{\partial E}{\partial R_{ks}} \right) \varepsilon_{13}(\mathbf{r}_s) + 2 \sum_k \left(\frac{y_{ks} z_{ks}}{R_{ks}} \frac{\partial E}{\partial R_{ks}} \right) \varepsilon_{23}(\mathbf{r}_s) \right]. \quad (4)$$

Following Glyde [15], we suppose that the rates of atom jumps in different directions are given by

$$\Gamma_i = \nu_i \exp\left(-\frac{Q_i}{k_B T}\right). \quad (5)$$

Here Γ_i is a rate of atom jump in i -direction, $Q_i = E_W - E_0$, is the activation barrier of atom transition in i -direction, where E_W is the potential energy of the system for the case when the atom comes to the saddle point and E_0 is the energy for the case when the atom is at equilibrium position, ν_i is a frequency factor.

It was shown, that equation (5) is right for a system under the displacement field [10].

The next moment of the approach is concerned with an evaluation of contributions in the change of the potential barrier $\Delta Q_i = Q_i - Q_0$, where Q_0 is the activation barrier for atom migration in a perfect lattice. The barrier for the atom jump is altered in accordance with equation (4) and $\Delta Q_i = \Delta E_W - \Delta E_0$. Now we not only take into account the change in the distance under strain between the jumping atom and its neighbors, but also the changes in the distances under strain between other atoms of the system (see for example, the distances presented by dashed lines in figure 1(a) and (b)).

The rate of atom jumps in different directions define the flux density of the vacancies, the explicit form of which can be derived by the ‘hole gas’ method suggested by Gurov [16]. This method allows us to calculate the balance of different jumps and their contribution to the flux. It is the main moment of the approach. More detailed descriptions of these steps can be found in [10, 11, 13].

3. Results

3.1. Vacancy diffusion under a stress. The FCC system

General equations for the components of the vacancy flux density for a given displacement field are

$$\begin{aligned} J_1 &= -\frac{1}{\Omega} \left[D_{11} \frac{\partial c}{\partial x} + D_{12} \frac{\partial c}{\partial y} + D_{13} \frac{\partial c}{\partial z} \right. \\ &\quad \left. - c \left(\frac{\partial D_{11}}{\partial x} + \frac{\partial D_{12}}{\partial y} + \frac{\partial D_{13}}{\partial z} \right) \right], \\ J_2 &= -\frac{1}{\Omega} \left[D_{21} \frac{\partial c}{\partial x} + D_{22} \frac{\partial c}{\partial y} + D_{23} \frac{\partial c}{\partial z} \right. \\ &\quad \left. - c \left(\frac{\partial D_{21}}{\partial x} + \frac{\partial D_{22}}{\partial y} + \frac{\partial D_{23}}{\partial z} \right) \right], \\ J_3 &= -\frac{1}{\Omega} \left[D_{31} \frac{\partial c}{\partial x} + D_{32} \frac{\partial c}{\partial y} + D_{33} \frac{\partial c}{\partial z} \right. \\ &\quad \left. - c \left(\frac{\partial D_{31}}{\partial x} + \frac{\partial D_{32}}{\partial y} + \frac{\partial D_{33}}{\partial z} \right) \right], \end{aligned} \quad (6)$$

where,

$$\begin{aligned} D_{11} &= \frac{D}{2} \exp\left(-\frac{K_1 \text{Sp}\varepsilon}{\theta}\right) \left[\exp\left(-\frac{K_2 \varepsilon_{33}}{\theta}\right) \text{ch}\left(-\frac{K_3 \varepsilon_{12}}{\theta}\right) \right. \\ &\quad \left. + \exp\left(-\frac{K_2 \varepsilon_{22}}{\theta}\right) \text{ch}\left(-\frac{K_3 \varepsilon_{13}}{\theta}\right) \right], \end{aligned}$$

$$\begin{aligned} D_{22} &= \frac{D}{2} \exp\left(-\frac{K_1 \text{Sp}\varepsilon}{\theta}\right) \left[\exp\left(-\frac{K_2 \varepsilon_{33}}{\theta}\right) \text{ch}\left(-\frac{K_3 \varepsilon_{12}}{\theta}\right) \right. \\ &\quad \left. + \exp\left(-\frac{K_2 \varepsilon_{11}}{\theta}\right) \text{ch}\left(-\frac{K_3 \varepsilon_{23}}{\theta}\right) \right], \\ D_{33} &= \frac{D}{2} \exp\left(-\frac{K_1 \text{Sp}\varepsilon}{\theta}\right) \left[\exp\left(-\frac{K_2 \varepsilon_{11}}{\theta}\right) \right. \\ &\quad \left. \times \text{ch}\left(-\frac{K_3 \varepsilon_{23}}{\theta}\right) + \exp\left(-\frac{K_2 \varepsilon_{22}}{\theta}\right) \text{ch}\left(-\frac{K_3 \varepsilon_{13}}{\theta}\right) \right], \\ D_{12} &= \frac{D}{2} \exp\left(-\frac{K_1 \text{Sp}\varepsilon}{\theta}\right) \exp\left(-\frac{K_2 \varepsilon_{33}}{\theta}\right) \text{sh}\left(-\frac{K_3 \varepsilon_{12}}{\theta}\right), \\ D_{13} &= \frac{D}{2} \exp\left(-\frac{K_1 \text{Sp}\varepsilon}{\theta}\right) \exp\left(-\frac{K_2 \varepsilon_{22}}{\theta}\right) \text{sh}\left(-\frac{K_3 \varepsilon_{13}}{\theta}\right), \\ D_{23} &= \frac{D}{2} \exp\left(-\frac{K_1 \text{Sp}\varepsilon}{\theta}\right) \exp\left(-\frac{K_2 \varepsilon_{11}}{\theta}\right) \text{sh}\left(-\frac{K_3 \varepsilon_{23}}{\theta}\right), \\ D_{21} &= D_{12}, \quad D_{31} = D_{13}, \quad D_{32} = D_{23}, \end{aligned} \quad (7)$$

where D is the vacancy diffusion coefficient in the perfect system, Ω is the atomic volume, c is the vacancy concentration, $\theta = k_B T$.

It should be emphasized that we did not assume that $K_2 \varepsilon_{ii}/\theta$ and the analogous ratios are small in contrast to the authors of [6] and some other works. One can readily see that in this case the vacancy flux density depends on the matrix of diffusion coefficients. Each of these coefficients depends on strain tensor components in a nonlinear way. In corresponding nonlinear equations, the functional dependence of strain is determined by coefficients, which are the main characteristics of the strain influence on diffusion (SID coefficients):

$$\begin{aligned} K_1 &= \sum_s \sum_{k \neq s} \left(\frac{(y_{ks}^W)^2}{R_{ks}^W} \frac{\partial E}{\partial R_{ks}} \Big|_{R_{ks}^W} \right) \\ &\quad - \sum_s \sum_{k \neq s} \left(\frac{(y_{ks}^0)^2}{R_{ks}^0} \frac{\partial E}{\partial R_{ks}} \Big|_{R_{ks}^0} \right) \\ K_2 &= \sum_s \sum_{k \neq s} \left(\frac{(x_{ks}^W)^2}{R_{ks}^W} \frac{\partial E}{\partial R_{ks}} \Big|_{R_{ks}^W} \right) \\ &\quad - \sum_s \sum_{k \neq s} \left(\frac{(x_{ks}^0)^2}{R_{ks}^0} \frac{\partial E}{\partial R_{ks}} \Big|_{R_{ks}^0} \right) \\ &\quad - \left[\sum_s \sum_{k \neq s} \left(\frac{(y_{ks}^W)^2}{R_{ks}^W} \frac{\partial E}{\partial R_{ks}} \Big|_{R_{ks}^W} \right) \right. \\ &\quad \left. - \sum_s \sum_{k \neq s} \left(\frac{(y_{ks}^0)^2}{R_{ks}^0} \frac{\partial E}{\partial R_{ks}} \Big|_{R_{ks}^0} \right) \right] \\ K_3 &= 2 \left[\sum_s \sum_{k \neq s} \left(\frac{y_{ks}^W z_{ks}^W}{R_{ks}^W} \frac{\partial E}{\partial R_{ks}} \Big|_{R_{ks}^W} \right) \right. \\ &\quad \left. - \sum_s \sum_{k \neq s} \left(\frac{y_{ks}^0 z_{ks}^0}{R_{ks}^0} \frac{\partial E}{\partial R_{ks}} \Big|_{R_{ks}^0} \right) \right]. \end{aligned} \quad (8)$$

These coefficients depend on the atomic interaction and atomic configuration of the defect environments such as when the atom comes to the saddle point (relative distances between the atoms have index W) and when the atom is at the equilibrium position (relative distances between the atoms have index 0). Equation (8) is obtained after consideration of the atom jump from the site with coordinates $(0, a/2, a/2)$ to the $(0, 0, 0)$ position. Analogical equations for other atom jump directions may be obtained with the help of a permutation of x, y, z in equation (8) taking into account a jump symmetry and the calculations of SID coefficients on the basis that all such equations give us the same values.

Accordingly, three coefficients K_1, K_2, K_3 determine the influence of the deformation field on the diffusion in a one-component system with an fcc structure.

3.2. Vacancy diffusion under a stress. The BCC system

The equation for the flux is the same as in the fcc structure, but the diffusion coefficients are different cardinally:

$$D_{11} = \frac{D}{2} \exp\left(-\frac{K_1 \text{Sp}\varepsilon}{\theta}\right) \left[\exp\left(+\frac{K_2 \varepsilon_{23}}{\theta}\right) \times \text{ch}\left(\frac{K_2(\varepsilon_{12} + \varepsilon_{13})}{\theta}\right) + \exp\left(-\frac{K_2 \varepsilon_{23}}{\theta}\right) \times \text{ch}\left(\frac{K_2(\varepsilon_{12} - \varepsilon_{13})}{\theta}\right) \right]$$

$$D_{22} = \frac{D}{2} \exp\left(-\frac{K_1 \text{Sp}\varepsilon}{\theta}\right) \left[\exp\left(+\frac{K_2 \varepsilon_{13}}{\theta}\right) \times \text{ch}\left(\frac{K_2(\varepsilon_{12} + \varepsilon_{23})}{\theta}\right) + \exp\left(-\frac{K_2 \varepsilon_{13}}{\theta}\right) \times \text{ch}\left(\frac{K_2(\varepsilon_{12} - \varepsilon_{23})}{\theta}\right) \right]$$

$$D_{33} = \frac{D}{2} \exp\left(-\frac{K_1 \text{Sp}\varepsilon}{\theta}\right) \left[\exp\left(+\frac{K_2 \varepsilon_{12}}{\theta}\right) \times \text{ch}\left(\frac{K_2(\varepsilon_{13} + \varepsilon_{23})}{\theta}\right) + \exp\left(-\frac{K_2 \varepsilon_{12}}{\theta}\right) \times \text{ch}\left(\frac{K_2(\varepsilon_{13} - \varepsilon_{23})}{\theta}\right) \right]$$

$$D_{12} = \frac{D}{2} \exp\left(-\frac{K_1 \text{Sp}\varepsilon}{\theta}\right) \left[\exp\left(+\frac{K_2 \varepsilon_{12}}{\theta}\right) \times \text{ch}\left(\frac{K_2(\varepsilon_{13} + \varepsilon_{23})}{\theta}\right) - \exp\left(-\frac{K_2 \varepsilon_{12}}{\theta}\right) \times \text{ch}\left(\frac{K_2(\varepsilon_{13} - \varepsilon_{23})}{\theta}\right) \right]$$

$$D_{13} = \frac{D}{2} \exp\left(-\frac{K_1 \text{Sp}\varepsilon}{\theta}\right) \left[\exp\left(+\frac{K_2 \varepsilon_{13}}{\theta}\right) \times \text{ch}\left(\frac{K_2(\varepsilon_{12} + \varepsilon_{23})}{\theta}\right) - \exp\left(-\frac{K_2 \varepsilon_{13}}{\theta}\right) \times \text{ch}\left(\frac{K_2(\varepsilon_{12} - \varepsilon_{23})}{\theta}\right) \right]$$

$$D_{23} = \frac{D}{2} \exp\left(-\frac{K_1 \text{Sp}\varepsilon}{\theta}\right) \left[\exp\left(+\frac{K_2 \varepsilon_{23}}{\theta}\right) \times \text{ch}\left(\frac{K_2(\varepsilon_{12} + \varepsilon_{13})}{\theta}\right) - \exp\left(-\frac{K_2 \varepsilon_{23}}{\theta}\right) \times \text{ch}\left(\frac{K_2(\varepsilon_{12} - \varepsilon_{13})}{\theta}\right) \right]. \quad (9)$$

For this structure, two coefficients K_1, K_2 determine the influence of the strain on the diffusion:

$$K_1 = \sum_s \sum_{k \neq s} \frac{(x_{ks}^W)^2}{R_{ks}^W} \frac{\partial E}{\partial R_{ks}} \Big|_{R_{ks}^W} - \sum_s \sum_{k \neq s} \frac{(x_{ks}^0)^2}{R_{ks}^0} \frac{\partial E}{\partial R_{ks}} \Big|_{R_{ks}^0}$$

$$K_2 = 2 \left(\sum_s \sum_{k \neq s} \frac{x_{ks}^W y_{ks}^W}{R_{ks}^W} \frac{\partial E}{\partial R_{ks}} \Big|_{R_{ks}^W} - \sum_s \sum_{k \neq s} \frac{x_{ks}^0 y_{ks}^0}{R_{ks}^0} \frac{\partial E}{\partial R_{ks}} \Big|_{R_{ks}^0} \right). \quad (10)$$

3.3. Diffusion under high pressure

In the case of a hydrostatic pressure P , with $\text{Sp}\varepsilon = -P/K_0$, $\varepsilon_{ii} = -P/(3K_0)$, $\varepsilon_{ij} = 0, i \neq j$ where K_0 is the bulk modulus. The expression for the vacancy flux density in the fcc system is

$$J^x = -\frac{D}{\Omega} \exp\left[\frac{P}{\theta K_0} \left(K_1 + \frac{K_2}{3}\right)\right] \frac{\partial c}{\partial x}, \quad (11)$$

where D is the vacancy diffusion coefficient under zero pressure.

Comparing the vacancy diffusion coefficient under pressure from equation (11) with its general thermodynamical expression [1], one gets the migration volume for fcc metals:

$$V^m = -\frac{1}{K_0} \left[K_1 + \frac{K_2}{3} \right] \quad (12)$$

and similarly in the case of bcc lattices:

$$V^m = -\frac{K_1}{K_0}. \quad (13)$$

As can be seen, the expression for the migration volume can be obtained in another way [15]. If we substitute the components of the deformation tensor corresponding to the case of the hydrostatic pressure into equation (4), we obtain the corresponding change of potential barrier ΔQ . (Since the system is now uniform, ΔQ_i for jumps performed in different directions are equal and the lower index can be deleted.) Substituting ΔQ in equation (5) for the jump rate, and taking into account that in the general case of random migration the diffusion coefficient D_R is related to the jump rate in a simple way [1]:

$$D_R = \frac{1}{6} \lambda^2 \Gamma, \quad (14)$$

where λ is the jump distance, we obtain the expression of the diffusion coefficient under pressure D_p :

$$D_p = \frac{1}{6} \lambda^2 \nu \exp\left(-\frac{Q_0}{\theta}\right) \exp\left(-\frac{\Delta Q}{\theta}\right) \quad (15)$$

and then for the migration volume:

$$V^m = -\frac{1}{6K_0} \left(\sum_k \sum_s R_{ks}^W \frac{\partial E}{\partial R_{ks}} \Big|_{R_{ks}^W} - \sum_k \sum_s R_{ks}^0 \frac{\partial E}{\partial R_{ks}} \Big|_{R_{ks}^0} \right). \quad (16)$$

Since we know K_1 and K_2 , it can be easily understood that both equations for volume migration are identical if the symmetry of the jumping atom coordinates is taken into account. These results are valid for the cases of vacancy diffusion in fcc and bcc structures.

The migration volume and SID coefficients are very sensitive to the atomic structure in the nearest vicinity of a defect and still more sensitive to the atomic structure of the saddle-point configuration. We have built an advanced model for their evaluation [17–19]. Some simulation results of mentioned structures in bcc metals and the migration volumes are presented in [17–19].

4. Summary

In the present paper, we proposed an original microscopic approach to examine how elastic strains of a general type affect the vacancy diffusion in the case of pure metals. The main physical ingredient of this approach is the fact that the positions of atoms are changed due to the displacement field and the potential energy of atoms is changed accordingly. This is true whatever the position of the atom under consideration is, in saddle as well as in an equilibrium configuration. We not only take into account a change in the distance under strain between a jumping atom and its neighbors, but also the changes in the distances under strain between other atoms in the system. General equations for the vacancy fluxes in fcc and bcc metals and new equations for SID coefficients are obtained. This generalization allows N-body potentials to be used for the calculation of the mentioned coefficients.

An application of the obtained equations in the case of a hydrostatic pressure gives us the possibility of determining the relation between the migration volume and SID coefficients in the fcc and bcc metals.

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