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Pressure Effects on Point Defect Diffusion Features in Cubic Metals. Atomic Simulation

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1. Introduction

We study pressure influence on point defect diffusive mobility. This permits to check-up the theories determining influence of elastic fields on diffusion fluxes because the diffusion under all-round compression conditions is the simplest process, which such influence becomes apparent into. Another important aspect of diffusion studies under high pressure is an opportunity to make choice between various possible mechanisms of diffusion in system. Unfortunately, there exist only a few experimental works dedicated to the study of pressure influence on diffusion. As to theory, microscopic calculations of volumes associated with defect migration are difficult. Calculations of migration volumes are few. We used a new approach, based on a molecular static method and taking into account the displacements of atoms in an elastic matrix around the computation cell. Using this method, the activation energies and activation volumes have been calculated for various metals with cubic structures.

2. Point defect diffusion feature simulation in cubic metals

In the framework of our model the atoms of a third zone are embedded in an elastic continuum and the displacements of these atoms ($\boldsymbol{u}$) are defined as a first ($\boldsymbol{u}_1$) and a second ($\boldsymbol{u}_2$) term in a spherical series expansion of the solution of the static isotropic elastic equation:

$$\boldsymbol{u}_1 = C_1 \frac{\boldsymbol{r}}{r^3},$$

$$\boldsymbol{u}_2 = C_2 \nabla \left[\frac{1}{r^5} \left(\frac{x^4 + y^4 + z^4}{r^4} - \frac{3}{5} \right) \right],$$

where $r = \left(x^2 + y^2 + z^2 \right)^{1/2}$ is the distance from the defect, C_1, C_2 – constants.

Previous calculations carried out for vacancy in bcc iron have shown that atomic displacements calculated using only first spherically symmetric terms of series don't agree with results of variation computations, even for sufficiently large outer limits of the system. This circumstance becomes apparent when the formation and migration volumes are estimated. Taking into account the second term of series allows to define atomic displacements in the elastic matrix more precisely and consequently equilibrium positions of all atoms in the vicinity of the defect are also defined more precisely.

We have performed a consistent iterative procedure to calculate the constants C_1 and C_2 and simulated the atomic structure in the crystal with a defect. The constants C_1 and C_2 calculated on a previous step of the iterative procedure are used to define the displacement of atoms in a third zone. Convergence of the iterative procedure is achieved.

Moreover, we take into consideration that the energy of the system (in particular the system with the defect) depends on the outer pressure. This dependence contributes to the values of migration and formation volumes [1]. The results show that the addition of this term in the formation volume is congruent to the usual one and in some cases exceeds it.

Furthermore, we take into account that the atom jumps into a vacancy in a time of a few oscillations in a lattice point. The displacement wave hasn't time to come to the crystal boundary and volume change as a whole doesn't take place. Consequently only the term, which concerns the pressure dependence of the system energy, contributes to the migration volume. To take this fact into account relaxation of only a part of atoms is performed. The relaxation range has been chosen on the grounds of results obtained by molecular dynamics simulations.

Using this method, the formation and migration volumes and the formation and migration energies have been calculated for various metals with cubic structures. Obtained diffusion features of point defects are studied depending on the number of atoms in the computation cell. In addition our model permits to calculate the temperature dependence of the mentioned features. We have evaluated the changes in the activation volume versus temperature.

3. Conclusion

A new model for simulation of point defect diffusion features is suggested. The substantial points of this model are as follows. First, we allow for displacements of atoms embedded in the elastic continuum around the computation cell. Second, we consider the influence of the discrete nature of the atomic structure in the vicinity of a defect on values and directions of atomic displacements in the elastic matrix. Third, we calculate the part of the activation volume concerned with the pressure dependence of the system energy. And at last, we take into account that an atomic jump into new position (when defect migrates) is a momentary process and therefore we carry out only partial relaxation in the vicinity of a defect.

The formation and migration energies and volumes have been calculated for vacancies, di-vacancies and interstitials in various metals with cubic structures using pair and many-body potentials. The obtained results confirm a stable convergence of the iteration procedure consisting in successive optimization of atomic structure near the defect and displacements of atoms in the elastic matrix. We have simulated diffusion features for various computation cell sizes and we have evaluated the temperature dependence of the formation and migration volumes.

References

[1] I.V. Valikova, A.V. Nazarov, A.A. Mikheev, Defect and Diffusion Forum 249 (2006) 55-60