diffusion-fundamentals

The Open-Access Journal for the Basic Principles of Diffusion Theory, Experiment and Application

Simulation of Diffusion under Pressure in BCC Metals

Irina Valikova, Andrei Nazarov

Department of Material Science, Moscow Engineering Physics Institute, Kashirskoe shosse, 31, 115409, Moscow, RUSSIA, E-Mail: Ivalikova@mail.ru

1. Introduction

One of the methods, which allows choosing the diffusion mechanism from several variants, is the study of the pressure influence on the diffusion coefficient. This influence is determined by the activation volume. However, microscopic calculations of volumes associated with defect migration are difficult. Calculations of migration volumes are few and they do not agree with each other and with the experimental results. In this paper, a new model for the simulation of the diffusion features of point defects is suggested. We used a new approach, based on a molecular static method and took into account the displacements of atoms in an elastic matrix around the computation cell.

2. Model for the simulation of the diffusion features of point defects

This work is devoted to the simulation of the diffusion features of point defects in bcc metals. It is known that the displacements of atoms calculated using the theory of elasticity solely are different from those obtained by means of simulation. These differences decrease with increasing distance from the defect (fig. 1).

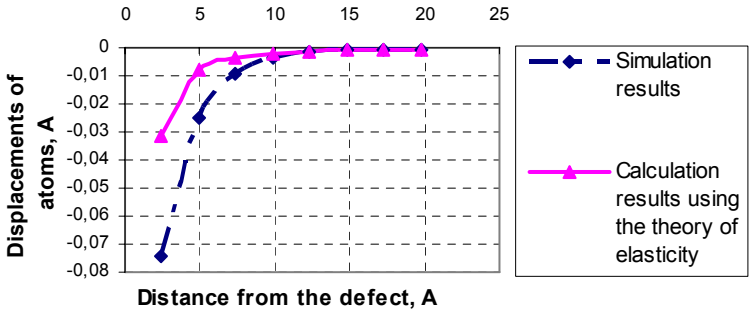

Fig. 1: Displacement of atoms in the vicinity of a defect.

The values of migration and formation volumes are very sensitive to the atomic structure in the vicinity of a defect, which makes it necessary to consider a large number of atoms in the computation cell and to take into account an elastic matrix around the cell. We have developed a new model taking these factors into consideration.

In the framework of this 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 solution of elastic equation:

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

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

where $r = \sqrt{x^2 + y^2 + z^2}$ is the distance from the defect, C_1, C_2 are constants.

The constants C_1 and C_2 are calculated by a consistent iterative procedure, and the atomic structure in the crystal with a defect is simulated. 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 and this procedure converges to a certain value after some iterations. Using this method, the formation and the migration energies E_v^f, E_v^m and the formation and the migration volumes V_v^f, V_v^m have been calculated for different bcc metals.

We studied the dependence of the displacement with a cubic symmetrical term in the solution of the elastic equation, i.e. with the constant C_2, on the distance from the defect. It turned out that for the vacancy this term does not give a noticeable contribution to the displacement if the computation cell has a sufficiently large size (about 20000 atoms in the computation cell).

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

3. Conclusion

A new model for simulating the diffusion features of point defects is suggested. The model is based on a molecular static method and takes into account the displacements of atoms in an elastic matrix around the computation cell. Convergence of the iterative procedure, which stabilizes the atomic structure in the vicinity of a defect, is obtained. With the help of this new model, the formation and the migration volumes have been calculated including contributions caused by the dependence of the energy of the system on the outer pressure. The obtained diffusion features of point defects are studied depending on the number of atoms in the computation cell.

References

[1] A.V.Nazarov**,** M.G.Ganchenkova, A.A. Mikheev, "Theory of diffusion under pressure", Defect and Diffusion Forum, Vol. 194-199, 2001, p 49.