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The Influence of Interstitial Impurity Atom – Vacancy Complex on Diffusivity of Interstitial Atom in α -Iron

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1. Introduction

This paper is devoted to simulation of the effect of interaction between impurity and point defect on interstitial atom diffusion.

In initial part the activation barrier set for different atomic configurations of impurity atom (i.e. carbon) and vacancy in α -iron have been calculated using a molecular static method (MS). In second part the diffusion coefficients depending on temperature have been calculated for carbon and vacancy in perfect lattice and in defect lattice using kinetic Monte-Carlo method (MC). Because of simulation results the anomalous diffusion of carbon in α -iron is analysed.

2. Model and simulation procedure

We consider a body-centered cubic lattice, in which there are two different types of point defects such as a vacancy and interstitial impurity atom.

The simulation consists of two steps:

- the calculation of the activation barriers for carbon atom and a vacancy in the different configurations of carbon–vacancy complexes,
- the simulation of carbon atom and vacancy migration and the calculation of carbon atom and vacancy diffusion coefficients depending on the temperature and the density of vacancies.

Molecular static method and calculation of the potential barriers. The aim of the MS-method is to determine the minimum energy configuration. In the present calculation about 1220 atoms surrounding the defect were treated as individual particles, each with three degrees of freedom. These atoms are represented as a spherical crystallite, which is located in the centre of atoms frozen at their perfect lattice positions. Atom interactions are described by potential functions for Me-Me and Me-C.

In this work, an empirical interatomic potential for the description of C interstitial impurity in metal is employed. Metal-metal interatomic potential of the EAM type is also used in simulation of metal interactions.

In the vicinity of a vacancy atomistic structure is distorted, and so equilibrium positions for metal atoms and carbon atom are determined by relaxation.

For the determination of the minimum energy configuration every atom of the central part is consecutively displaced as long as the energy of this atom reaches a minimum value. Then, also the total energy of the system reaches a minimum. This procedure is called relaxation. Then we move one of the atoms from its equilibrium position to a vacant nearest-neighbor equilibrium position step by step. At the same time we relax the

system and calculate the moving atom energy and total energy on every step. Consequently the activation barrier for an atom jump is obtained.

Monte-Carlo method and determination of the diffusion coefficients. Using the values of the activation barrier which are obtained with the help of the MS-method the jump rates are calculated as:

$$\Gamma_i = \nu \exp[-(Q_0 + \Delta Q_i) / (k_B T)], \quad (2)$$

where Γ_i is the frequency of an atom jump in i -direction; ν is a frequency factor; Q_0 is the activation energy for atom migration in a perfect lattice; ΔQ_i is the change of the activation energy for atom migration in a lattice with point defect (in the i -direction); k_B is Boltzmann's constant; T is the temperature. On basis of these data the atom migration are simulated by using the MC-method.

The mean distance is calculated in every experiment after a certain number of trials K . Then the root-mean-square displacement $\langle R_K^2 \rangle$ is calculated for different temperatures and averaged over a certain number of experiments (where R_K is the distance between the initial position of the migrating atom and its final position in trial K). The diffusion coefficient is obtained by Einstein's formula:

$$D = \langle R_K^2 \rangle / (6t) \quad (3)$$

and

$$t = K \Delta \tau, \quad (4)$$

where t is the migration time which is much more than the mean time between jumps of the atoms ($\Delta \tau$). The relation of the diffusion coefficients is calculated as:

$$D_{\text{def}} / D_{\text{p.l.}} = \langle R_K^2 \rangle_{\text{def}} / \langle R_K^2 \rangle_{\text{p.l.}}, \quad (5)$$

where $D_{\text{p.l.}}$ and $\langle R_K^2 \rangle_{\text{p.l.}}$ are the carbon diffusion coefficient and the root-mean-square displacement of the carbon in the perfect lattice; correspondingly, D_{def} and $\langle R_K^2 \rangle_{\text{def}}$ are the carbon diffusion coefficient and the root-mean-square displacement of the carbon in the lattice with point defects, respectively.

3. Results

Thus we calculated a set of activation barriers for the jumps of atoms in different directions and different configurations of the carbon-vacancy complex by the MS-method.

The diffusion coefficients for vacancy and carbon migration are simulated in the perfect lattice and in a lattice with point defects (i.e. vacancies) by the MC-method using the set of activation barriers. We computed the diffusion coefficients of carbon in dependence on the temperature and the vacancy density.

The vacancy and the carbon atom migrate as a bonded complex in a definite temperature range. In this case the mechanism of a dynamic couple is realised and an acceleration of carbon diffusion is observed. This allows to interpret the anomalous diffusion of carbon in α -iron at high temperatures.

4. Conclusion

We have developed a model taking into consideration that point defects can alter the surrounding atom configuration and the local magnitude of the activation barrier for interstitial atomic jumps. The simulations reveal an acceleration of carbon diffusion.