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Simulation of Pressure- and Temperature Dependence of Impurity Diffusion in BCC Metals

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1. Introduction

Pressure influence on diffusion is a very important problem but unfortunately it is insufficiently studied. Especially, the substitutional impurity diffusion should be noted. In our work a new approach is suggested. This approach is based on Manning's "five-jump" model for impurity diffusion and on our computer model, which permits to determine potential barrier heights for vacancy jumps in various directions relative to impurity as well as respective migration volumes. Our approach allows us to calculate the temperature- and pressure dependences of impurity diffusion coefficient taking into account correlation effects.

2. A New Approach for Impurity Diffusion Study

Some time ago Manning et al. [1] have developed the theory for the evaluation of a impurity diffusion correlation factor ("five-jump model"). Correlation factor f as well as diffusion coefficient is expressed through the rates of vacancy jumps in various directions with respect to impurity w_1, w_2, w_3, w_4 [1]:

$$f = \frac{1+C}{1-C}, \quad C = \frac{-w_2}{w_2 + 2w_1 + 3.375w_3 + \left[\frac{w_1 w_4}{w_1 + w_4}\right]} \tag{1}$$

However in that time there was no approach allowing to estimate these jump rates.

Recently we developed a model [2] for calculation of point defect diffusion features in metals, which permits to simulate vacancy jumps with respect to impurity atom and allows us to calculate potential barrier heights and respective migration volumes for these jumps as well as their temperature dependences. Thus the combination of Manning's theoretical approach and our computer model allows to obtain temperature- and pressure dependences of features of various jumps. Therefore it gives an opportunity to calculate the impurity diffusion coefficient versus temperature and pressure taking into account the correlation effects. A novelty of our approach lies therein.

In our model a new algorithm is realized that makes it possible to self-consistently determine atomic structure near defect and constants characterizing the displacement of the atoms in an elastic matrix around computational cell. We take into account that the atom jumps into the vacancy for the time of a 1-2 oscillations in the lattice point and so we carry out the relaxation of only those atoms which are located in a distance less than five lattice parameters from the defect. Such a distance was chosen on the grounds of the results obtained by the molecular dynamics method [2].

The results of molecular dynamics showed that a geometrical similarity of the atomic structure in the vicinity of the defect remains with temperature changes. In other words, the distances between atoms in the system with the defect change proportionally to the coefficient of thermal expansion in the same way as they change in the ideal system [3]. This fact permits us to use our model developed earlier for calculation of temperature dependence of point defect diffusion features in metals.

Vacancy jumps in BCC iron in the various directions relative to copper impurity atom were simulated using our model. The temperature dependence of corresponding migration volumes (Fig. 1) and potential barrier heights were obtained. So we calculated the impurity diffusion coefficient versus temperature and pressure taking into account temperature dependence of migration volumes and estimated the activation volumes for copper impurity diffusion in iron.

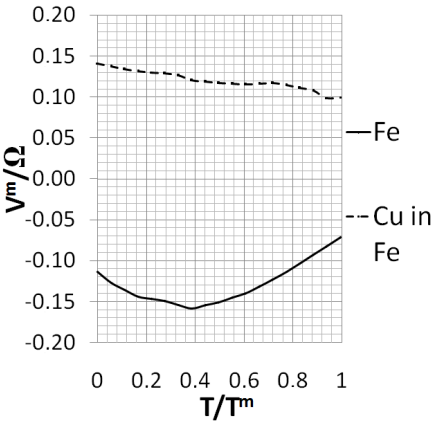

Fig. 1: Vacancy migration volume in BCC iron and migration volume for copper impurity atom jump versus temperature.

3. Conclusion

A new approach for pressure- and temperature dependence of impurity diffusion in BCC metals study is suggested in this work. This approach is based on Manning's "five-jump" model for impurity diffusion and on our computer model. In our model a new algorithm is realized that makes it possible to determine atomic structure near defect and takes into account that the atom jumps into the vacancy for the time of a 1-2 oscillations in the lattice point.

Vacancy jumps in BCC iron in the various directions relative to copper impurity atom were simulated using our model. Taking into account that geometrical similarity of the atomic structure in the vicinity of the defect remains with temperature changes the temperature dependence of corresponding migration volumes and potential barrier heights were obtained. Using above-mentioned results we calculated the copper impurity diffusion coefficient versus temperature and pressure as well as activation volumes for copper impurity diffusion in iron.

References

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