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N-Body Potentials in Simulation of Point Defect Properties

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1. Introduction

It is known that in a vacancy diffusion mechanism, dominant in pure metals, the main diffusion properties are the vacancy formation and migration energies E_v^f, E_v^m and the formation and migration volumes V_v^f, V_v^m

$$D = D_0 \exp\left(-\frac{E_v^f + E_v^m + V_v^f p + V_v^m p}{kT}\right). \quad (1)$$

However, there are no good methods for calculation of the activation volume, defining the influence of pressure on the diffusion coefficient. This work is devoted to this problem with the new approach.

One of the main problems of the modern computer simulation is to choose a realistic way of interatomic interaction. Unfortunately, with the simplicity, the pair-potential model has serious drawbacks [1]. In this work we used the Finnis-Sinclair formalism [1,2] of N-body interactions, free from disadvantages of pair potentials for the atomic structure calculations near defects and receiving the diffusion properties described above.

2. Object and method of simulation

We have found that the activation volume is extremely sensitive to the atomic structure in the vicinity of a defect, so it is very important to calculate the most correct atomic positions. To achieve this purpose, we have developed a new approach, based on a molecular static method giving the opportunity to simulate point defect properties with the usage of N-body potentials. In the framework of new approach, the bulk is divided into three concentric zones. Atoms of the third, external zone are embedded in an elastic continuum. So, we used an iterative procedure, including simulation to define the atomic displacements in the immediate vicinity of a defect, calculation of constant C in the second zone according to the first term of the elastic equation solution $\boldsymbol{u}=C\boldsymbol{r}/r^3$ and the following atomic displacement near the bulk border, in the third zone. We have found a stable convergence of constant C and atomic positions in several (about 10) steps. Then the relaxation volume has been calculated with the equilibrium magnitude of constant C:

$$\Delta V_{rel} = \iint u dS = 4\pi C \quad (2)$$

Moreover, we have taken into consideration that the energetics in crystal depends on pressure. And it is different for ideal and defective bulk. These pressure-dependent terms of the activation volume have been calculated using the approach presented in [4]. Most simulations don't appreciate this term, but the results obtained show that its value is congruous to the usual one and in some cases exceeds it.

2. Results

The characteristics, obtained for some metals are performed in the following table. The special interest was to study both normal and anomalous metals, and to compare the results for these cases. Also we perform a comparison of the results, obtained for N-body and pair-potentials.

The diffusion properties obtained for α-Fe and β-Zr.

	α-Fe		β-Zr
	N-body, Ackland [2]	Pair-pot., Johnson	WM1 [3]
E_v^f, эВ	1,70	2,91	1,55
E_v^m, эВ	0,79	0,69	0,32
E_v^{SD}, эВ	2,49	3,78	1,87
$\Delta V_{rel}/\Omega$	-0,159	-0,132	-0,472
$\Delta V_p^{E_f}/\Omega$	0,021	0,015	0,014
V_v^f/Ω	0,862	0,854	0,542
$\left(\Delta V'_{rel}-\Delta V^0_{rel}\right)/\Omega$	0,009	0,011	10^{-4}
$\Delta V_p^{E_m}/\Omega$	0,041	-0,032	0,089
V_v^m/Ω	0,050	-0,022	0,089
V_v^{SD}/Ω	0,912	0,832	0,631

3. Conclusion

The diffusion properties obtained are in a good agreement with the existing experimental data. The new approach allowed to attain the most fine structure in the vicinity of a defect, and consequently to perform a more accurate calculation of activation volumes. It is also necessary to accent that N-body potentials give more adequate results, especially in cases of the formation energy and the pressure-dependent term of the migration volume for Fe.

References

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