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Molecular Dynamics Simulation of Atomic Structure in the Vicinity of Point Defects in FCC and BCC Metals

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1. Introduction

Experimental data indicates that features determining pressure dependence of point defect concentration and diffusivity, are temperature-dependent [1]. For the theoretical description of such dependence knowledge of atomic structure at finite temperatures is needed. Thus the aim of our work is a detailed study of temperature-defined changes of atomic structure surrounding vacancies and self-interstitials, as the changes in structure do affect these features. In this work Molecular Dynamics (MD) is applied to determine atomic structure in the vicinity of point defects at different temperatures. This enables the calculation of temperature dependence of these features, based on atomic structure obtained via Molecular Statics (MS) [2].

2. Model Description and Results

Atomic structure of different FCC and BCC metals is studied by MD using velocity Verlet algorithm. Free boundary conditions are applied with the ball-shaped cell. To decrease surface effects up to 40000 atoms are used. Various pair and many-body potentials for Al, Cu, Ni, Fe, V are used. Coordinates of the central atom and its neighbors are averaged during a simulation, which time (400 and up to 1000 atomic vibrations) is considered sufficient enough. We use the obtained mean positions of atoms to directly calculate interatomic distances. Thus, as the result of calculation, we get the temperature dependence of lattice parameters and of distances between atoms inside its four nearest lattice shells in a system with the point defect. As a result of our simulation we found that the ratio of these distances in a system with defect to lattice parameter remains constant with temperature (Fig. 1).

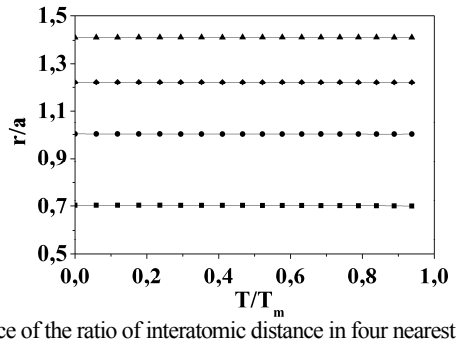

Fig. 1: Temperature dependence of the ratio of interatomic distance in four nearest coordination spheres to the lattice parameter in FCC Al (—■— r_1/a —●— r_2/a —◆— r_3/a —▲— r_4/a)

This leads to the essential assumption, that the ratio of any interatomic distance in the vicinity of the point defect to the lattice parameter doesn't change with temperature, e.g. the ratio is constant. Therefore geometrical similarity of atomic structure in the vicinity of point defects preserves in spite of the changes in temperature. Through this similarity any distances between atoms nearby point defects can be calculated at every temperature having only these distances at 0 K and the thermal expansion coefficient.

This fact makes it possible to get the temperature dependence of energy and volume of point defect formation. These features are calculated according to distances between atoms and interatomic interaction. Initial atomic positions, e.g. at 0 K, are determined by the MS method. Formation energy and volume of point defects at 0 K are calculated the same way taking into account correspondent positions of atoms. Recalculation of interatomic distances at every temperature results in temperature dependence of formation energy and volume. Simulation results for vacancy formation energy and vacancy formation volume are given in Table 1.

Table 1.

T/T_m	Al		Cu		Ni		α-Fe		V	
	E_f^v,eV	V_f/Ω	E_f^v,eV	V_f/Ω	E_f^v,eV	V_f/Ω	E_f^v,eV	V_f/Ω	E_f^v,eV	V_f/Ω
0.1	0.68	0.50	1.21	0.65	1.54	0.98	1.71	0.76	2.52	0.88
0.3	0.68	0.51	1.22	0.72	1.54	1.02	1.71	0.80		
0.5	0.69	0.52	1.22	0.79	1.54	1.05	1.72	0.86	2.52	0.84
0.6	0.70	0.53	1.22	0.82	1.54	1.07	1.72	0.90	2.52	0.81
0.7	0.70	0.53	1.23	0.84	1.53	1.10			2.52	0.80
0.8	0.71	0.55	1.23	0.87	1.52	1.12			2.53	0.79
0.9	0.72	0.56	1.23	0.89	1.50	1.14			2.53	0.77
Exp.	0.67	0.62	1.28	0.75	1.79	0.8	1.79	0.95	2.2	-

3. Conclusion

We've achieved the result of geometrical similarity preservation in the vicinity of point defect, that works both in case of FCC and BCC metals. According to this fact features of point-defects, that depends on atomic structure, can be obtained at finite temperatures.

References

[1] F.J. Kedves, G. Erdelyi, Defects and Diffusion Forum, 66–69 (1989) 175–188.

[2] I. Valikova, A. Nazarov, Phys. Met. Metallography, 105 (2008) 578–586.