Computer modeling of atomic clusters formation in grain boundaries

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Atomic interaction in grain boundaries (GB) leads to the complexes formation. Up to now two types of the complexes were analyzed for binary systems with restricted solubility: A_mB_n for systems with intermediate phases and B_2 – without them [1]. It was shown that effect leads to the increase of segregation and decrease of diffusivity.

There are no direct experimental data on the complexes in GB, only indirect results, obtained by molecular dynamics modeling [2]. The author used model of GB containing 18000 Al atoms. The part of them was replaced by Fe atoms. With the use of the half-empiric potential Al-Fe it was shown that in the Al-based alloy with 2.5 at.% Fe, in symmetric GB (100) the complexes of Fe_2-type are formed and the coordination number Fe-Fe is close to 1,that is much more than in random distribution. It was also shown that the complexes formation leads to decrease of mean-square atomic displacements and therefore of diffusion coefficient.

At the present study we investigated the mobility of the copper atoms. Model of 269640 atoms contained two symmetrical GB's sigma 5 (001) (012). For a few pairs of accidental atoms near the grain boundary, placed on 2.6 nm from each other, the energy of interaction (dipole energy, ΔE_{dipole}) between the atoms was introduced, as well as the energy of segregation at GB (ΔE_{seg}). The mean square displacement of atoms within 100 ns at 1000 and 1200 K was measured (Fig.1)
The data on displacment were recalculated to diffusion coefficients. (Table 1)

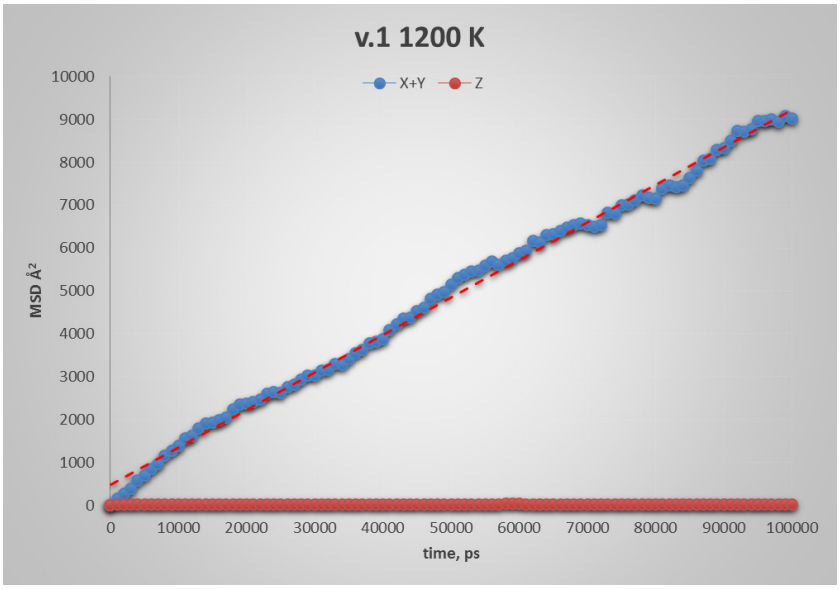

Fig.1 - Typical dependence of the mean square displacement of pairs of atoms vs time.

Table 1 - Data of dipole energy, energy of seregation and diffusion coefficients

V	ΔE_{dipole} eV/atom	ΔE_{seg} eV/atom	D cm²/s	
			1000	1200
v.1	-0,059	0,008	3,94E-07	2,19E-06
v.2	-0,199	0,006	2,08E-07	1,46E-06
v.3	-0,497	0,014	4,01E-08	1,03E-07
v.3	-0,063	0,478	2,06E-07	9,47E-07
v.5	-0,285	0,463	5,94E-08	4,87E-07

It is seen from the table the diffusion coefficients decrease with increasing the dipole interaction energy and segregation energy.

Conclusions.

A formation of the atomic complexes in GB is possible in systems with restricted solubility. The complexes formation leads to decrease of mean-square atomic displacements.

1 Esin V., Bokstein B.S., Rodin A.,O., Grain Boundary Diffusion Model in B-regime with regard to the formation of atomic complexes in grain boundaries. Def. and Dif. Forum, vol 309-310 (2011) pp. 29-38

2 Mendelev M.I., Rodin A.O., Bokstein B.S. Computer simulation of Fe diffusion in liquid Al and along Al grain boundaries. Def. and Dif. Forum, vol 309-310 (2011) pp. 223-230