Atomic interaction in grain boundaries and related phenomena

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Atomic segregation at grain boundaries (GB), as a result of atoms interaction with GBs, has a prolonged history [1]. The fact that grain boundary diffusion (GBD) is moderated under the action of grain boundary segregation (GBS) is now generally recognized.

Meanwhile, at the case of heterodiffusion, except of atoms interaction with GB, it is necessary to take into account atoms interaction between them in GB. Such interaction leads to the formation of atomic complexes. This conclusion is based on the results of thermodynamic study [2,3] and results of computer simulation which showed the possibility of B2 type complexes formation in Fe-Al system, a deviation of solute-solute coordination number from random distribution [4] and decrease of mean square atomic displacements (MSD) [5]. The last effect can be possibly connected with recently observed absence of the accelerated GBD Fe and Co in Cu compared with bulk diffusion [6,7].

At the present talk the peculiarities were studied of grain boundary self diffusion in Cu connected with the effect of atomic pairs formation in GBs.

The molecular dynamics (MD) simulation of GB selfdiffusion was used taking semiempirical potential designed for Cu [8,9]. To be sure in adequacy of the model proposed, the double product (δD_{gb}, where δ is a width of GB and D_{gb} is a coefficient of GB selfdiffusion) of GB selfdiffusion was obtained based on MSD of free atoms at different temperatures (825, 900, 1000 and 1200K).

The results obtained for δD_{gb} and D_{gb} (δ is taken as 0,5 nm) are in a good agreement with experimental results [10,11] and other results of computer simulation [12] taking into account a difference in chosen potentials and types of GBs.

The results are compared with similar simulation but with artificial addition the energy of interaction (E) between identical atoms in arbitrary chosen pairs. To obtain reliable data on the MSD at comparatively low temperatures the used simulation cell consists of three thousands atoms, two symmetrical GBs Σ5 (001)(012) and 70 pairs of identical random Cu atoms in GBs

bonded into pairs. It was required also that MD should run at least 100ps.

It was shown that the complexes formation leads to decrease of MSD for atoms bonded into the pair compared with free atoms. The pair interaction energy E=-0,2 eV/atom influences only slightly on D_{gb} which decreases to 15-45% comparing with E=0. The activation energy changes in limits of error. At E=-0,5 eV/atom Dgb decreases more than at order of magnitude and activation energy increases at 1,5 times comparing with E=0.

The results obtained involve also dependence the number of the stable pairs on time and temperature and show the possibility of pairs to condense into ternary, quarterly and more numerous complexes.

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