Computer simulation of atomic complexes formation in grain boundaries

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For the molecular dynamics simulation of grain boundary selfdiffusion (GBSD) in Cu the embedded atom method (EAM) potential was used, obtained in [1], was used. The calculations were performed for the special grain boundary (GB) Σ5 (012)[100]. The mean square displacement (MSD) and GBSD coefficients were calculated. The results are in a good agreement with experimental results [2] and other results of computer simulation [3].

For description of grain boundary heterodiffusion (GBD) the next method was proposed. Into the model contained GB, close to GB symmetry plane, the marked M-atoms of hypothetical impurity were artificially added. These M-atoms are completely identical with other Cu atoms, but interact with the pair interaction energy Ea. After, the model was annealed for a long time at temperatures from 900 to 1200 K.

It was shown that for Ea=0.0 eV/atom MSD and GBD coefficients coincide with the GBSD values. For Ea=-0,2 and -0,5 eV/atom a decrease of MSD values and GBD coefficients was observed. It is supported, that such effect is connected with two reasons: the atoms moving from GB to the bulk and complexes formation from two and more atoms. The diffusivity of atoms in bulk, as well as diffusivity of the complexes are negligibly small. The "free" atoms move as in a pure Cu. Hence, a decrease of diffusivity is connected with a decrease of the movable atoms, but not with their mobility.

References.

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