ENERGETICALLY FAVORABLE CONFIGURATIONS OF SYMMETRIC GRAIN BOUNDARIES TILT IN HCP-TITANIUM

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Materials

In this work, the structure and energy of the grain boundaries symmetric tilt [2-1-10] were investigated in hexagonal titanium. The energies of the formation of point defects are obtained for various atomic sites in the grain boundaries. The main purpose of this work was to determine the structure of the most stable grain boundaries alpha-titanium by molecular statics modeling. The existing deviations from the lattice theory of the coincidence site lattice (CSL) for hexagonal close-packed (hcp) metals, therefore, studying the structure of grain boundaries for some hcp metals are relevant. The point defects in our study are self interstitial atoms (SIA) and vacancies.

Methodology

Static configurations grain-boundary structures (GB) were obtained, using the molecular statics (MS) method. The GB formation energy $E_{gb}$ was determined as:

$$E_{gb} = (E_p - (N_0E_{coh}))/2S,$$

where $E_p$ is the total potential energy of the system, $N_0$ is the number of atoms in the system, $E_{coh}$ is the cohesion energy (binding energy per lattice atom of an ideal crystal), $S$ is the GB area. The presence of two boundaries takes into account the doubled area $S$ in the denominator. The vacancy(SIA) energy was calculated as the energy required to remove(formation) an atom at a certain position of the GB and create(remove) an atom in an ideal lattice infinitely distant from the GB, according to the formula:

$$E_{v,SIA} = E_f - (N_0\pm1)^*\left(E_i/N_0\right),$$

where $E_f$ is the initial energy of the system, before the removal(formation) of an atom, $N_0$ is the total number of atoms, $E_i$ is the energy of the system after the removal(formation) of an atom, and $N_0\pm1$ particles, $\pm$" for vacancy, "$\pm$" for SIA. The term $E_i/N_0$ is the energy per atom.

The point defect formation energies are calculated specifically for each system. The energy per atom is about 1% different from the coupling energy and energy per atom calculated for each system.

Results


Examples of the dependence of the energy of vacancy formation on the distance from the boundary are shown below.

Structures GB, misorientation angle 64.3°. Asterisk indicates the place where the SIA will be inserted. The minimum energy of SIA formation for this boundary is 0.5012 eV.

Conclusions

A computer simulation of the structure and energy of symmetric tilt [2-1-10] boundaries has been performed for polycrystalline titanium. A grain-boundary structure (misorientation angles of 64.3° and 86.62°) was found, containing point defects. The resulting configurations corresponded to the minimum formation energy and were found by molecular statics methods. The dependences of the vacancy energy on the distance to the plane of the boundary are given. The data allows you to estimate the GB width and show the GB positions most likely to accommodate point defects. The study was supported by a grant of Russian Science Foundation No. 21-13-00063.

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