3 - 14 Molecular Dynamics Simulation of Cu Atoms Interaction with Symmetrical Grain Boundary of BCC Fe

Gao Ning, Wei Kongfang and Wang Zhiguang

The symmetrical GB Σ3{112} of BCC Fe with Cu atoms is relaxed firstly with MS-MD-MS process in order to understand the possible segregation phenomena of Cu atoms in bcc Fe. The interactions between Cu atoms with symmetrical Σ3{112} GB in BCC iron have been simulated with MD and MMC methods based on the recently developed Fe-Cu empirical potential. Only two atomic layers belonging to the GB are identified by CNA method after full MS-MD-MS relaxations with Mendelev potential 2. The defect-pair (Cu-V) binding energies in GB are found to be close to the values in the bulk perfect BCC iron. Binding energy of Cu_m to GB is positive and increases with increasing the size of cluster, indicating the absorption of these clusters to GB. In GB, the energy calculations show that absorbed Cu-V clusters prefer to form larger clusters with low number density instead of randomly distributed high number density state. The 3D structure is found to have lower energy when the size of Cu-V cluster is large, which can also undergo the phase transition from BCC to FCC with radius larger than 2.5 nm. After the phase transition of the precipitate, the high atomic stress up to 30 Gpa has been found around the crack tip on the GB plane. The local configuration after MMS and MD simulations is shown in Fig. 1 together with the displacement of relative atoms involved in the phase transtion. It is therefore believed that Cu atoms can segregate to the GB plane and affect the mechanical properties of the materials.

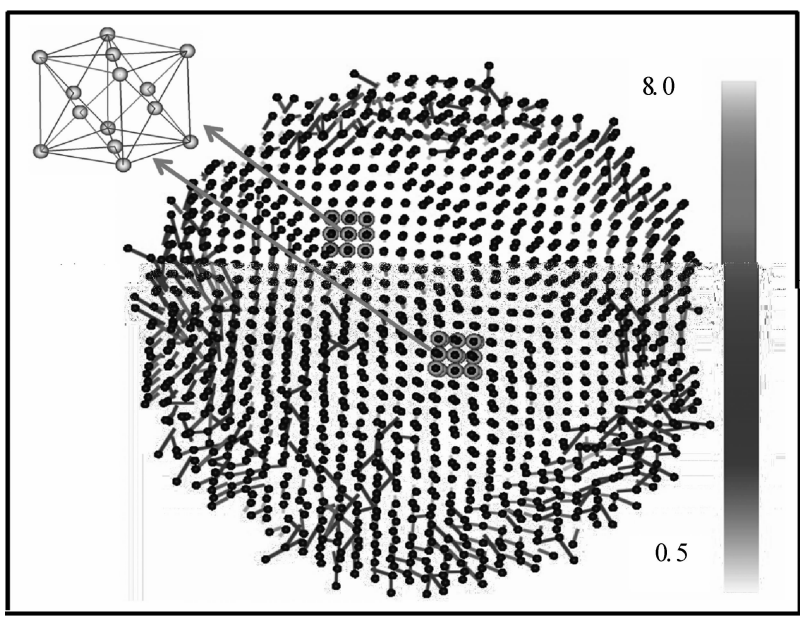

Fig. 1 The displacement of each Cu atom on the cross section containing the phase transition after full relaxation in the precipitate with radius of 2.5 nm. The value of each displacement is identified by the color-map from 0.5 to 8 Å. The example of formed FCC lattice is shown in the inset picture.