3 - 16 Energy State and Phase Transition of Cu Clusters in BCC- Fe Studied by a Molecular Dynamics Simulation

Gao Ning, Wei Kongfang, Zhang Shixu and Wang Zhiguang

The behavior of copper atoms (Cu) in body-centered cubic iron (bcc Fe) has an important effect on the properties of Fe-alloy since the very low solubility of Cu in Fe, leading to the formation of Cu precipitate during the relaxation process. When the size of cluster is small, the coherence has been found experimentally between the Cu precipitate and BCC Fe matrix. While the size of such cluster increases, the phase transition would be expected to occur for Cu precipitate, leading the incoherence at the interface between them. Thus, the embrittlement initially from these incoherences is expected. In order to understand fully such phenomena, the energy should be firstly calculated for different state of Cu atoms within the small and large clusters with the different number distribution. The phase transition is then identified as the size of precipitate increases. In this paper, the molecular static (MC) and dynamics (MD) simulations method was used for such purpose with Fe-Cu many-body potential. A new method named common neighbour analysis (CNA) has also been used to describe the phase transition process.

Three different energy states of Cu atoms in bcc Fe were calculated, as shown in Fig. 1. For these 3 cases, the total Cu atoms are same, that is, 160 Cu atoms bcc Fe but in different state. The energy of the whole system has then been calculated for these three cases, showing the total energy of system decreases when the size of cluster is larger. Thus, the Cu atoms prefer to clustering in bcc Fe.

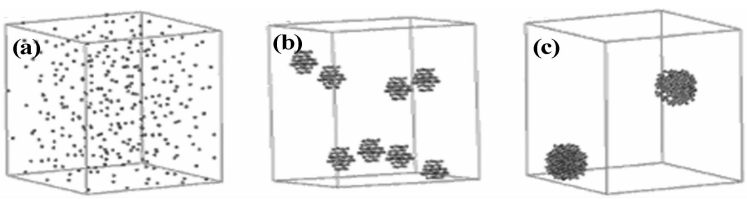

Fig. 1 Three types of initial Cu clusters in bcc Fe. The small particles are Cu atoms. (a) The Cu atoms are distributed randomly and individually in bcc Fe. The Cu atoms are in cluster state but with different number, 40 and 160 Cu atoms in each cluster in (b) and (c), respectively.

As the size of the Cu precipitate increases to around 3.0 nm, the phase transition has been observed. The results are analyzed by CNA method to identify the region in which the bcc lattice structure has been changed to fcc. In Fig. 2, the region identified by CNA and alto together with the displacement of these atoms are shown. The formed fcc lattice is also shown in the figure. The formed fcc Cu precipitate structure has the lattice constant of 3.54 angstrom, which is close to the value of perfect fcc Cu lattice.

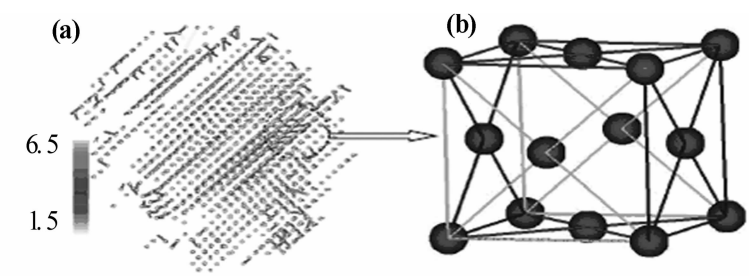

Fig. 2 (a) The Cu atoms in the form of fcc lattice structure after phase transition indicated by the CNA method. The displacements of these atoms are also shown by the short lines characterized by the color map with the range from 1.5 to 6.5 angstrom. The local formed fcc structure is shown in (b).

In summary, the energy state of the Cu cluster in the bcc Fe matrix has been calculated, indicating that the Cu atoms prefer to form a cluster instead of being uniformly distributed in the Fe-Cu system. The binding energy of substitutional Cu to Cu cluster shows that the acceleration of the ripening process may occur from the cluster with around 30 Cu atoms. The phase transition is found to be related with the local stress state induced by the vacancies surrounding the precipitate. The formed fcc Cu precipitate structure has the lattice constant of 3.54 angstrom, which is close to the value of perfect fcc Cu lattice.