3 - 17 Molecular Dynamic Simulation of Cu Segregation at Fe Grain Boundary

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Impurity segregation at grain boundaries (GB) is one of the significant effects on the mechanical properties of alloys, e. g. , embrittlement and cracking. Experiments on the Reactor Pressure Vessel (RPV) steel and Fe-Cu alloys indicate that Cu-rich clusters produced by irradiation play an important role in the hardening and embrittlement of materials[1]. The very low solubility of Cu atoms in bcc Fe may also trigger the segregation of Cu atoms at grain boundary in Fe matrix and affect the mechanical properties of materials. Computer simulation of segregation at GB at atomic scale can provide such valuable insight for understanding these micro-processes. In the present work, the Cu atom segregation process at Fe symmetrical grain boundary $\sum 5(012)$ was chosen and investigated with molecular dynamics(MD) method for such purpose.

Three Fe GB $\sum 5(012)$, containing 184320, 40000 and 23040 Fe atoms respectively, were created by using Coincident Site Lattice (CSL) theory. The Fe-Cu potential used in the simulation was developed by Pasianot and Malerba[2]. After relaxation, with the system potential $E^{\text{tot}}(\text{GB})$ and the total areas of GB A, the formation energy of GB E^{f}_{GB} can be calculated by:

$$E^{\text{f}}_{\text{GB}} = \frac{E^{\text{tot}}(\text{GB}) - NE^{\text{Fe}}}{2A}$$

where, N is the total number of atoms in GB, E^{Fe} is the energy of single Fe atoms in BCC perfect lattice. The calculated formation energies with the different size simulation boxes are approximately the same, 0.0871 eV/Å^2. Thus, the case with 40000 atoms in the box is enough for further calculation in the work.

In GB with 40000 Fe atoms, ten substitutional Cu clusters with different distances to GB, from 0 to 57.2 , were chosen to calculate the system energy as the function of the distance between the Cu cluster and the GB. In each Cu cluster, 10 Cu atoms are included by replacing according Fe atoms, as shown in Fig. 1. Small points are Fe atoms, the larger are substitute Cu atoms, the horizontal line indicates the GB plane. The potential energies of these systems are calculated by MD simulations. After simulation, the segregation energies of Cu clusters can be calculated and the results for the case containing 10 Cu atoms in the cluster are shown in Fig. 2.

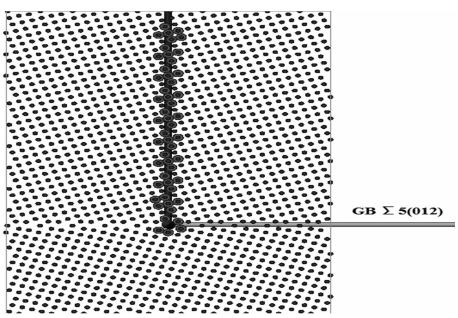

Fig. 1 10 Cu clusters in GB system.

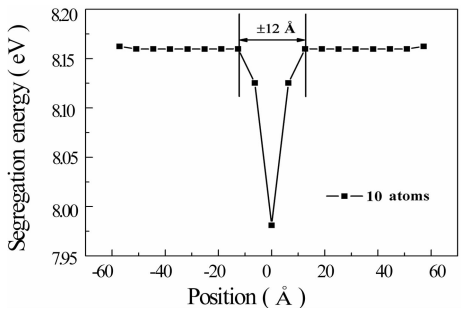

Fig. 2 Segregation energy of Cu clusters with 10 atoms.

From Fig. 2, it can be found that the total energy of system increases rapidly with the distance of Cu cluster far away from the GB regions, from 0 to ±12 Å, and then shows a constant after 12 Å. When the size of Cu clusters increases to 20 and 30 atoms, similar phenomena are also observed, implying that the impact of GB $\sum 5(012)$ is limited in a certain range, less than 12 Å for such symmetrical GB.

From above results, the conclusion can be made that the Cu atoms prefer to segregate at GB region by decreasing the total energy of the system. The driven force is from the very low solubility of the Cu atoms in bcc Fe matrix. When the size of the Cu cluster in the GB increases, our previous work has confirmed bcc to fcc lattice structure phase transition, leading to an increase of local stress. Thus, the embrittlement of Fe-Cu alloy can be expected to occur earlier in GB than in bulk.

References

[1] G. R. Odette, G. E. Lucas. JOM, 53, 7(2001)18.
[2] R. C. Pasianot, L. Malerba. Journal of Nuclear Materials, 360, 2(2007)118.

3 - 18 Nano-hardness of Chinese RAFM Steel Irradiated with Energetic Kr, Xe and Bi Ions

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In the present work, nano-indentation hardness of Chinese RAFM steel irradiated with Kr, Xe and Bi ions at different temperature were investigated. The energetic Kr, Xe and Bi ions irradiation experiment was performed at the materials research terminal of 320 kV Multi-discipline Research Platform for Highly Charged Ions. Kr, Xe and Bi ions with a kinetic energy of 4, 5 and 6 MeV were used for the irradiation, respectively. The ion beam was raster scanned by using two sets of triangle wave generator electric source installed at the front beam line, with scanning frequencies of 1.0 kHz and sanning voltage 0.8 kV in the horizontal direction and 1.0 kV in the vertical direction, respectively.

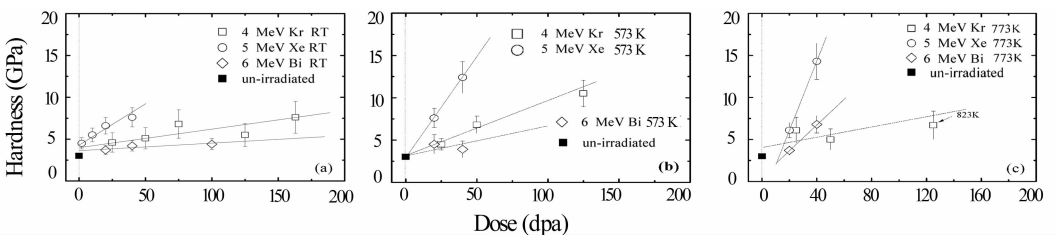

Fig. 1 Peak nano-hardness of Chinese RAFM steel irradiated with Kr, Xe and Bi ions as a function of damage level at different temperatures: (a) RT; (b) 300℃; (c) 500℃.

After irradiation, nano-hardness of the samples was investigated by using MTS corporation G200 nano-indenter. The nano-indentation measurements were performed by using a triangular pyramid Berkovic indenter. Nano-hardness profiles were obtained by a contact pressure evaluation method. Fig. 1 gives the peak nano-hardness of Chinese RAFM steel irradiated with Kr, Xe and Bi ions as a function of damage level at different temperatures. Each data point in the nano-indentation graph represents the peak hardness corresponding to peak damage region at the end of energetic ions projectile ranges. Based on the analysis of nano-hardness results, it shows that the nano-hardness of irradiated Chinese RAFM steel increases obviously with increasing of irradiation dose and temperature. At the same temperature, there is an approximate linear relationship between nano-hardness and irradiation dose. With temperature increasing, nano-hardness as a function of irradiation dose increases more quickly. The maximum value (~15 GPa) of nano-hardness appears in Chinese RAFM steel irradiated with 5 MeV Xe ion at 500℃ to dose of 40 dpa. The nano-hardness of Chinese RAFM steel results suggest that there is obviously a close relationship between nano-hardness and irradiation ions, dose and temperature. The different kinds of defects induced by irradiation may play an important role in the slip process of dislocation line and resulted in the nano-hardness increase.