§ 5. Modeling of Irradiation Performance and Fundamental Data for Fusion Materials

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Modeling of materials behavior is not only the mechanistic understanding of macroscopic irradiation effects from short and fine scales of phenomena but also providing the critical methodology for the quantitative estimation of the reliability of the irradiated materials for long term operation. Behaviors of materials used in severe neutron irradiation environment should be estimated either by materials database or materials simulation code to design first wall/blanket structures. In this study, behavior of defect clusters during deformation is discussed based on the current progress of molecular dynamic simulation study.

(1) Molecular Dynamic Simulation of Glissile Interstitial Clusters during Deformation

Irradiation induced hardening of metal and alloy is characterized by an increase of the yield stress of irradiated materials with increasing irradiation dose and decreasing irradiation temperature [1-6]. The increase in yield stress is due to the interactions of the dislocations responsible for the plastic deformation with the irradiation defects. According to the recent Cascade Induced Source Hardening (CISH) mechanism [1], the glissile interstitial clusters generated directly from cascade process are considered to play a controlling role for the hardening and yield drop phenomena. Such mechanism was also supported by some TEM observation where decoration of defects was observed near dislocations. To model the irradiation hardening by this mechanism, two important aspects must be clarified. One is the decoration parameter, for example the standoff distance; the other is the unpinning process of dislocation from decoration. Trinkaus et al. have examined the central question of the formation of dislocation decoration [2] and provided analytical estimates for elastic interactions between small defect clusters and an infinite long, straight edge dislocation. However, their analysis was based on elasticity theory, which is only suitable for long-range interactions. For short-range interactions, molecular dynamics should be used to supply atomistic resolution processes. Recently, Rodney and Martin [3] investigated the interaction between glissile interstitial clusters and dislocations in nickel by MD simulations and supplied such atomistic interaction process for the first time. However, copper and stainless have a much lower stacking fault energy than nickel. It is still not clear on the influence of the low SFE character. On the other hand, prismatic slipping, which has always been used in explaining the elimination mechanism of Frank loop [10-14], has never been clarified at atomistic resolution detail in spite of its importance.

For deformation simulation in FCC metals, which involve twining, it is very important to use atomic potentials that can correctly reproduce the stability of FCC against HCP and BCC structure. In this study, Long-range EAM potentials (Mishin [4]) were used for its advantage in that aspect. The calculation model consisted of about 120,000 atoms of 30x33x30 a_0. Verlet integration algorithm [5] was used for integrating the controlling equations of MD.

Figure 1 shows an example of MD simulation of interaction stages of 7-SIA glissile clusters and extended dislocation near the yielding points during deformation. The upper cluster glided one-dimensionally along the partial dislocation even at the extremely low simulation temperature at 10^{-6} K. At the same time, the mobility of partial dislocation decreased and the dislocation segment bow-out due to pinning.

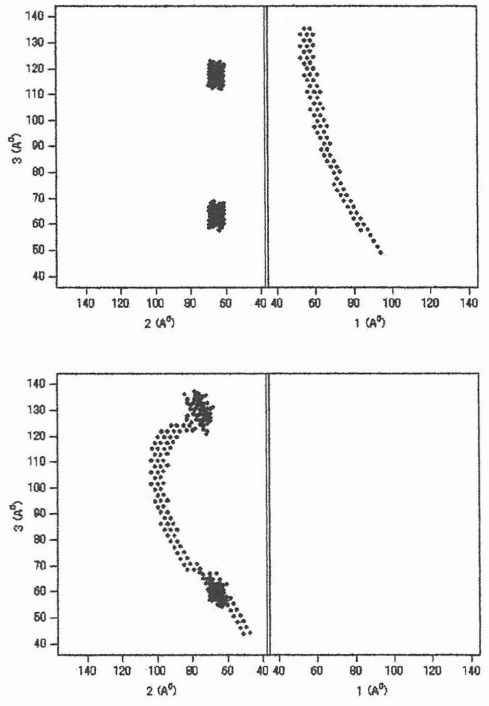

Fig. 1 A sequence of interaction of 7-SIA clusters and extended dislocation during deformation in Cu.

References

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