A study to evaluate the interaction between glissile loops in BCC systems

Y. Yunmin\textsuperscript{a}, T. Okita\textsuperscript{b} and N. Sekimura\textsuperscript{b}

\textsuperscript{a}Dept. of Quantum Engineering & System Science, Graduate School of Engineering, Tokyo University, 7-3-1 Hongo, Bunkyo-ku, 113-8656 Tokyo, Japan

\textsuperscript{b}UNIVERSITY OF TOKYO, 7-3-1 Hongo, Bunkyo-ku, 113-8654 Tokyo, Japan

okita@q.t.u-tokyo.ac.jp

The 14MeV neutrons generated by fusion produce high-energy collision cascades. Recent MD simulations show that self-interstitial atoms produced in these cascades directly agglomerate into small dislocation loops, and many of them are glissile in nature. These small loops will subsequently diffuse and interact with other loops or network dislocations. As a result, the formation of larger loops as well as the evolution of the network dislocations depends also on the capture rate of these small loops rather than of individual self-interstitials only. In BCC alloys, the migration energies are very low even for the large loops, and the interaction between loops are one of the controlling steps for the microstructural evolution under irradiation.

In this study, we evaluated the interaction between $a_0\{111\}/2$ loops, which can be often observed in BCC systems, and calculated the stable positions along the glide cylinder of the loop by the elastic theory. In this calculation, we include the change in the normal vector and the rotation of the loop to minimize the interaction energies.

The rotation of the loop under the strain field of the other loop is not so significant at far distance, because of its short-range interaction. Whether the loop attracts another loop or not depends on the spatial relation and the combination of the Burgers vector of them. The Molecular Dynamics simulations are also conducted to compare the results obtained from the elastic theory.