Contribution ID: **28** Type: **contributed**

Simulation of interaction between dislocations and hydrogen/helium in tungsten

Thursday, 18 July 2024 12:10 (20 minutes)

Tungsten is considered one of the most promising plasma materials for future fusion reactors. In the fusion reactor environment, the irradiation of high-energy neutrons leads to material collisions, generating vacancies and interstitial atoms, such as Frankel defects. These microscopic defects gradually evolve into larger-scale complex defects, such as dislocations and dislocation loops, through diffusion and aggregation. These linear defects often form simultaneously during material fabrication and irradiation, and they can absorb point defects, thereby influencing their processes of aggregation and annihilation. Furthermore, dislocation defects have the ability to capture hydrogen or helium atoms, affecting their penetration and retention behavior, thereby impacting the safe operation of fusion reactors.

Atomic-scale simulation methods, including molecular statics and molecular dynamics, are employed to systematically study the interactions between dislocations in tungsten and point defects, hydrogen, and helium atoms. This includes (1) the interaction and migration behavior of two types of point defects in tungsten: 1/2<111> screw dislocations and vacancies/self-interstitial atoms (SIAs) along the <111> direction; (2) the interaction and diffusion behavior of hydrogen/helium atoms with 1/2<111> screw dislocations and 1/2<111>{110} edge dislocations in tungsten; (3) the interaction and diffusion behavior of hydrogen/helium atoms with 1/2<111> interstitial dislocation loops in tungsten; (4) the synergistic effects of dislocations and helium clusters on hydrogen atoms.

These simulation results contribute to a deeper understanding of the mechanisms by which intrinsic dislocations in tungsten affect defect evolution and the penetration and retention behavior of hydrogen and helium atoms. Furthermore, they provide input parameters for larger-scale computational simulations and offer theoretical support for explaining experimental phenomena. These research findings provide crucial theoretical support for explaining experimental observations of the aggregation of defect clusters, hydrogen bubbles, and helium bubbles near dislocations.

Primary author: LI, Xiaochun (Institute of Plasma Physics, Chinese Academy of Sciences)

Co-authors: LUO, Guang-Nan (Institute Of Plasma Physics, Chinese Academy Of Sciences); ZHOU, Haishan (Institute of Plasma Physics, Chinese Academy of Sciences)

Presenter: LI, Xiaochun (Institute of Plasma Physics, Chinese Academy of Sciences)

Session Classification: PSI and PMI modelling