Summit to: Monte Carlo Methods in Computational Materials Science

Multiscale Dynamic Modeling of Displacement Damage in Metal under Neutron Irradiation

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EXTENDED ABSTRACT: Intense neutron irradiation can cause severe displacement damage to metal components, causing key problems such as thermal/mechanical degradation [1]. Accurately understanding, predicting and regulating the irradiation damage behavior is key to improve the anti-irradiation ability of materials. Therefore, a sequential multiscale simulation platform was established for modeling displacement damage in metal, by developing the accelerated cascade-annealing model (IM3D) [2], the short-term defect dynamic evolution model (MMonCa) [3] and the long-term defect dynamic evolution model with time-space-correlation (IRadMat) [4]. The evolution of displacement defects in Fe/W-based metals under neutron irradiation and its effect on the macroscopic properties of materials were studied, which are consistent with experiments. It shows that: 1) The intra-cascade time-space correlation effect greatly affects the long-term evolution and size distribution of defects, which dominates the displacement damage behavior in materials. 2) Neutron pre-irradiation damage as new sinks of H/He aggravates the H/He retention and surface damage near the surface [5]. This provides theoretical guidance for the selection/design of new radiation resistant metals and the analysis/prediction of their displacement damage effects.

Keywords： multiscale dynamics modeling; displacement damage; metals; spatial correlation; neutron irradiation

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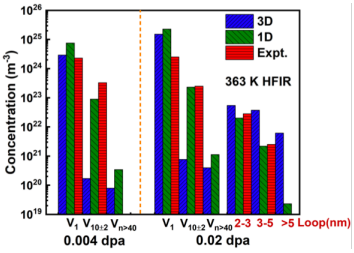

Figure 1. comparison of defect size distributions between CD simulations and the experiment in single crystal tungsten under the HFIR fast neutron irradiation condition.

BIOGRAPHY

Qi-Rong Zheng is a doctoral candidate of Condensed Matter Physics in Institute of Solid State Physics, Chinese Academy of Sciences and University of Science and Technology of China. She has participated in the publication of more than 6 papers in the field of multiscale modeling of material radiation damage in nuclear materials.

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