Commun. Comput. Phys.
doi: 10.4208/cicp.030311.090611a

Vol. **11**, No. 5, pp. 1547-1568
May 2012

A Cluster Dynamics Model for Accumulation of Helium in Tungsten under Helium Ions and Neutron Irradiation

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Received 3 March 2011; Accepted (in revised version) 9 June 2011

Communicated by Haiqing Lin

Available online 3 January 2012

Abstract. A cluster dynamics model based on rate theory has been developed to describe the accumulation and diffusion processes of helium in tungsten under helium implantation alone or synergistic irradiation with neutron, by involving different types of objects, adopting up-to-date parameters and complex reaction processes as well as considering the diffusion process along with depth. The calculated results under different conditions are in good agreement with experiments much well. The model describes the behavior of helium in tungsten within 2D space of defect type/size and depth on different ions incident conditions (energies and fluences) and material conditions (system temperature and existent sinks), by including the synergistic effect of helium-neutron irradiations and the influence of inherent sinks (dislocation lines and grain boundaries). The model, coded as IRadMat, would be universally applicable to the evolution of defects for ions/neutron irradiated on plasma-facing materials.

PACS: 02.60.Cb, 61.80.Az, 61.72.Cc, 61.72.J-

Key words: Cluster dynamics model, rate theory, helium and neutron irradiation, tungsten, accumulation and diffusion.

1 Introduction

In tokamak fusion reactors (e.g. ITER), plasma-facing materials (PFMs, e.g. Be, C and W) suffer heavy bombardment from the plasma by particles such as hydrogen isotope

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(H, D and T) and helium (He) ions with the energy ranging from 10 eV to several keV as well as energetic neutrons and high heat loads generated by D-T fusion reaction [1]. This process can cause damages to the metal surface, such as, erosion, sputtering, blistering, etc. [2]. Especially, He atoms injected into metals would be deeply trapped by lattice defects such as vacancies and He-vacancy complexes formed by themselves or neutrons irradiation [3], which can alter the microstructure and thus the mechanical properties of the material. On the other hand, due to their excellent thermal properties, low solubility for hydrogen and low sputtering yield, tungsten (W) based materials are termed as potential candidates for the divertor armor tiles in the future fusion reactor like ITER [2]. Therefore, the mechanisms of defects accumulation and diffusion under He ions irradiation on PFMs like W are important to estimate the damage formation and distribution, which have not been well understood.

Consequently, effects of He ions irradiation on W and other metals have been extensively investigated over a wide range of burning plasma conditions with different ion energies/fluences and system temperatures, using ion accelerators or large-sized plasma confinement devices as well as several analysis techniques [3–25]. During implantation, injected He atoms would be deeply trapped by different kinds of existing lattice defects near surface. Thus, the distribution of He atoms in W is mainly in near surface of several nms to several- tenth nms for keV He ions, while a little fraction can extend into in-bulk. It is necessary to comprehend the mechanics of He trapping and diffusion effects and the contributions by different types of He clusters in W quantitatively.

While the evolution of defects upon irradiation is by nature a multi-scale phenomenon, numerical study of defects evolution requires a multi-scale atomistic-continuum modeling approach [26, 27]. Particularly for the long-term kinetic evolution of defects, cluster dynamics (CD) [25, 28] and kinetic Monte Carlo (KMC) models [29, 30] are commonly used by requiring previous knowledge of defects created during irradiation, their mobility as well as their energetic properties [31]. These models have also been performed to the case of He ions irradiation on W, recently. Watanabe et al. [25] studied the formation of interstitial loops in W under He ions irradiation by using rate theory modeling and compared with experiment. Xu et al. [28] investigated the effects of He on the microstructure evolution in W during He and neutron irradiations based on a simple model using rate theory. Perhaps, more reliable parameters (especially the characteristic energies) or more reasonable reaction mechanisms of defects should be addressed to obtain credible results. Becquart et al. [29, 30] studied the micro-structural evolution of irradiated W with He by using an object KMC (OKMC) model based on the ab initio parameterizations. However, this model can not be applied to the case of long-range scale diffusion due to its low efficiency.

In fact, although KMC model can account for the spatial and temporal correlations, it is limited to small volumes ($\sim \mu m$), low irradiation dose (typically much less than 1 dpa) and small time scales, far from the order of practical nuclear reactor undergoing. On the contrary, CD model based on the mean-field rate theory can explore the evolution of defects over large space scales (intermediate-length) and time scales ($\sim \mu s$ to years),