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Rate theory modeling of dislocation loops in RAFM steel under helium ion irradiation and comparison with experiments

Yanxia Yu [a], Xinfu He [b], Fengfeng Luo [a], Liping Guo [a,*]

[a] Hubei Nuclear Solid Physics Key Laboratory and School of Physics and Technology, Key Laboratory of Artificial Micro- and Nano-structures of Ministry of Education, Wuhan University, Wuhan 430072, China

[b] China Institute of Atomic Energy, Beijing 102413, China

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ABSTRACT

A modified model based on kinetic rate theory is presented to simulate the dose dependence of defects nucleation and growth in reduced-activation ferritic/martensitic (RAFM) steel under helium ion irradiation by considering the motion of dislocation loops. The modeling results are compared with the transmission electron microscopy (TEM) experiments. The TEM analysis shows that the mean size of dislocation loops increases with the increasing atomic displacement damage dose, while the density of the observed loops exhibits minor change. To investigate the evolution of dislocation loops, we compare two cases incorporating mobile and immobile interstitial clusters in our modified model, respectively. The calculated results reveal a good agreement with experiments in the case of considering mobile interstitial clusters. It is included the motion of interstitial clusters plays an important role in the evolution of dislocation loops in RAFM steel.

1. Introduction

It is well known that the issue of serious irradiation damage in materials is one of the main factors impeding the development of fusion reactors as a long-term energy source [1,2]. High-energy fusion neutrons will cause various irradiation effects such as hardening, swelling and an increase of ductile-brittle transition temperature, which may greatly influence the lifetime of fusion reactors [3,4]. In spite that a variety of experiments have been conducted for observation of these phenomena, there are still some limitations for initial stages during the formation of defects within $\sim 10^{-9}$ s and problems regarding the evolution of single point-defects are remained. Therefore modeling plays an important role in theoretical analysis due to its convenience and effectiveness for solving these problems. The rate theory is one of the fruitful modeling methods capable of treating the long term kinetic evolution of microstructures in metals under irradiation [5–7]. To build up the rate theory model, it is essential to understand the detailed evolution of defects. In model, defects are distinguished by their associated properties, for instance, size, migration energy, binding energy and so on, and reactions between them are described in the form of a set of differential equations, which can only be solved numerically. Due to its low computational cost, rate theory is one of the best ways to reproduce the real interactional processes of defects, and can allow investigations under different conditions using the large number of inputs [8].

RAFM steels have been proposed as one of the main candidates for the first wall structural materials in fusion reactors owing to its good properties under fusion conditions [9]. In fusions reactors, the first wall structural materials simultaneously suffer from high-energy neutrons irradiation and transmuted helium and hydrogen irradiation, yielding a substantial number of defects, like vacancies, interstitial atoms, dislocation loops and voids. The freely migrating interstitials will interact with each other, to allow the formation of dislocation loops which will cause transgranular embrittlement [10]. Understanding the issue of time development of dislocation loops in the presence of helium will help us to know better about the factors which influence the evolution of dislocation loops [11–14]. Related theoretical studies have reported some progresses in the effects of interstitial clusters in RAFM steels based on rate theory [15,16,22–24]. Hardouin Duparc et al. studied the nucleation and growth of point-defect clusters of ferritic model alloys under 1 MeV electron irradiation using the results from experiments and found that the existence of copper in iron is capable of stabilizing interstitial clusters [15]. Meslin et al. had investigated the process of defect clusters producing in α-iron under krypton ion irradiation condition by considering the mobility of point-defect clusters [16]. But there are seldom explorations focusing on the

* Corresponding author. Tel.: +86 27 6875 2481x2223; fax: +86 27 6875 2569.
E-mail address: guolp@whu.edu.cn (L. Guo).

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dose dependence evolution of interstitial clusters in RAFM steels under helium ion irradiation.

In recent years there are a series of theoretical and experimental studies exploring the defect dynamics in metals, which are produced by high-energy particles irradiation, including the glide processes of interstitial clusters containing several to thousands of interstitials [17–21]. In earlier models, people only consider the production and removal of point defects from defect clusters for simplification, since this kind of simplified model can also satisfy demands in certain situations. But questions about whether and how the interstitial type dislocation loops larger than nanometer size move keep confusing for a long time. Molecular dynamics (MD) study revealed that clusters containing a few interstitials exhibit one-dimensional diffusion in the form of migration and diffusivity pre-factors [17]. However, due to the time limitation of MD method, the mobility of larger clusters is seldom studied, although it was experimentally observed by TEM as reported in some literatures [18–20]. It is worth to note that the diffusion process of dislocation loops larger than 5.9 nm in diameter was observed by Arakawa et al., and was given in formulistic form of diffusion factors [18]. Recently, Xu et al. systematically explored the discrepancy in defect clusters evolution between models considering mobile interstitial clusters and immobile ones under the same conditions respectively, and found a significant difference in density and size of interstitial clusters [21]. It is clear that mobile interstitial clusters play an important role in model description for theoretical study. Therefore, under the condition of ion irradiation, there exists at least a part of interstitial clusters exhibit mobility.

In the present work, we also study dislocation loops by TEM analysis under 30 keV helium ion irradiation at 450 °C. Meanwhile, the nucleation and growth of dislocation loops is explored using kinetic rate theory under different irradiation time and doses, which enable us to compare directly with experiments. The rate theory model used by Yoshiie et al. to investigate the kinetic evolution of defects in ferritic and austenitic steels is modified by introducing the interaction between mobile interstitial clusters, in order to get better description about the dose dependence of defect evolution under helium ion irradiation at high temperature [22].

2. Experimental

This work was performed on reduced activation martensitic steel (namely SCRAM steel) provided by Huazhong University of Science and Technology with a composition of 9.24% Cr, 2.29% W, 0.49% Mn, 0.25% V, 0.25% Si, 0.088% C, 0.0059% P in wt.%, and Fe for balance [25]. The samples were prepared by twice quenching and tempering processes, including quenching at 1253 K for 0.5 h, tempering at 1033 K for 2 h, and then quenching at 1233 K for 0.5 h, tempering at 1013 K for 2 h. 0.5 mm thick plates were cut from bulk materials, and were then mechanically polished to about 0.1 mm thick. The 3 mm diameter standard TEM discs were punched out from these plates, and milled into a thickness of 40∼50 μm with silicon carbide paper of grades 800–2500 at the final milling stage. Standard TEM disk specimens were polished and thin foils were prepared using 5% perchloric acid and 95% ethanol polishing solution at −30 °C by a MTPA-5 twin-jet electropolishing machine which was produced by Shanghai Jiaotong University.

TEM thin foils were irradiated with 30 keV helium ions on an ion implanter in the Accelerator Laboratory of Wuhan University. Temperature was maintained at 450 °C, which was monitored with a thermocouple, within an error of ±5 °C during irradiation. Detailed irradiation conditions were listed in Table 2. The irradiated helium fluence are 1.6×10^{15}, 5×10^{15}, 1.3×10^{16} and 2.5×10^{16} cm^{-2} respectively, corresponding to peak damage dose of 0.1, 0.3, 0.8 and 1.5 dpa respectively. The damage dose and the helium concentration were calculated in detailed cascades by SRIM2008 with 40 eV displacement energy as recommended in ASTME521-89 [26]. Classical TEM observations were performed in a JEM-2010HT TEM operated at 200 kV, below the threshold energy for knock-on damage in iron. The TEM images were taken under bright-filed (BF) imaging conditions.

3. Model description

The rate theory model is based on a mean field approach, which accounts for the evolution and reaction between defects, as well as the nucleation and growth of interstitial clusters, vacancy clusters and bubbles, and the sink strength for mobile defects are simultaneously considered. The concentration and radius in the rate equations are averaged over all the defects respectively. The formulated model includes the basic types of defects as follows: self-interstitials (I), vacancies (V), helium atoms (He), self-interstitial clusters (IC), void (VC), vacancy–helium pairs (V,He), bubbles (B). The vacancy–helium pair mentioned above denotes one helium atom in one vacancy. Bubbles are defined as vacancy clusters with helium. Here di-interstitials and di-vacancies are regarded as the nucleus of interstitial type dislocation loops and voids respectively, which can formed directly in cascades. The thermal dissociation is only considered for vacancy–helium pairs.

The following rate equations describe the rate of concentration change of interstitials, vacancies and helium,

$$\begin{aligned}\frac{dC_I}{dt} &= P_I(1-\varepsilon_R)(1-\varepsilon_I) - 2Z_{I,I}M_IC_I^2 - Z_{I,V}(M_I+M_V)C_IC_V \\ &\quad - Z_{I,IC}M_IC_IS_I - Z_{I,VC}M_IC_IS_V - Z_{I,B}M_IC_IS_B - Z_{I,VHe}M_IC_IC_{V,He} \\ &\quad - M_IC_IC_S - \langle N_I\rangle P_{IC}, \end{aligned} \tag{1}$$

$$\begin{aligned}\frac{dC_V}{dt} &= P_V(1-\varepsilon_R)(1-\varepsilon_V) - 2Z_{V,V}M_VC_V^2 - Z_{I,V}(M_I+M_V)C_IC_V \\ &\quad - Z_{He,V}(M_{He}+M_V)C_VC_{He} - Z_{V,VC}M_VC_VS_V - Z_{V,IC}M_VC_VS_I \\ &\quad - Z_{V,B}M_VC_VS_B - M_VC_VC_S + M_{He}T_{V,He}C_{V,He} \\ &\quad - Z_{V,VHe}M_VC_VC_{V,VHe} - \langle N_V\rangle P_{VC}, \end{aligned} \tag{2}$$

$$\begin{aligned}\frac{dC_{He}}{dt} &= P_{He} - Z_{He,V}(M_{He}+M_V)C_VC_{He} - Z_{He,VC}M_{He}C_{He}S_V \\ &\quad - Z_{He,B}M_{He}C_{He}S_B - Z_{He,VHe}M_{He}C_{He}C_{V,He} + Z_{I,VHe}M_IC_IC_{V,He} \\ &\quad + M_{He}T_{V,He}C_{V,He} - M_{He}C_{He}C_{SHe}. \end{aligned} \tag{3}$$

In order to account for the nucleation of interstitial clusters, vacancy clusters, vacancy–helium pairs and bubbles, a set of rate equations are structured as, respectively,

$$\frac{dC_{IC}}{dt} = P_I(1-\varepsilon_R)\varepsilon_I/\langle N_I\rangle + Z_{I,I}M_IC_I^2 - k_L^2C_{IC}^2, \tag{4}$$

$$\frac{dC_{VC}}{dt} = P_V(1-\varepsilon_R)\varepsilon_V/\langle N_V\rangle + Z_{V,V}M_VC_V^2 - Z_{He,VC}M_{He}C_{He}S_V, \tag{5}$$

$$\begin{aligned}\frac{dC_{V,He}}{dt} &= Z_{He,V}M_{He}C_VC_{He} - Z_{V,VHe}M_VC_VC_{V,He} - Z_{I,VHe}M_IC_IC_{V,He} \\ &\quad - M_{He}T_{V,He}C_{V,He} - Z_{He,VHe}M_{He}C_{He}C_{V,He}, \end{aligned} \tag{6}$$

$$\frac{dC_B}{dt} = Z_{V,VHe}M_VC_VC_{V,He} + Z_{He,VC}M_{He}C_{He}S_V + Z_{He,VHe}M_{He}C_{He}C_{V,He}, \tag{7}$$

where P is production rate of Frenkel pairs in cascades. ε_R is the fraction of defects recombined in cascades. ε_I and ε_V are the fractions of interstitial clusters and vacancy clusters formed directly