Fusion Engineering and Design 137 (2018) 303–311

Contents lists available at ScienceDirect

Fusion Engineering and Design

journal homepage: www.elsevier.com/locate/fusengdes

Mesoscale modeling of irradiation damage evolution in bcc iron and vanadium: A comparative study

Yuanyuan Wang[a], Jianhua Ding[a], Shaosong Huang[a], Jijun Zhao[a,*], Yunzhi Wang[b]

[a] Key Laboratory of Materials Modification by Laser, Ion and Electron Beams (Ministry of Education), Dalian University of Technology, Dalian, 116024, China
[b] Department of Materials Science and Engineering, The Ohio State University, Columbus, OH, 43210, USA

ARTICLE INFO

Keywords:
Irradiation
Void
Dislocation loop
Phase field
Rate theory

ABSTRACT

Voids and dislocation loops are two major types of damages in irradiated structural materials, which are mainly responsible for the degradation of material properties. Here we use the phase-field model and rate theory to simulate the microstructural evolution of voids and dislocation loops, respectively, in irradiated bcc iron and vanadium. The temperature-dependent material parameters of iron and vanadium are derived from *ab initio* calculations. The simulated results at different temperatures (513 K, 623 K and 722 K) and irradiation doses (1 ~ 20 dpa) are analyzed to reveal the impact of irradiation conditions on the formation of irradiation-induced defect clusters. A comparison of the results shows larger void porosity and void/loop size in iron and higher void/loop density in vanadium. Then, a dispersed-barrier hardening model is used to correlate the mesoscale simulation results on microstructure with the yield stress change of the materials.

1. Introduction

Numerous Frenkel pairs are generated within the primary knocked-on atom (PKA) cascade in a structural material subjected to high-energy particles irradiation [1]. Vacancies and self-interstitials diffusion, recombination and aggregation result in the formation of defect clusters (e.g., voids and dislocation loops). Such irradiation damages lead to hardening, swelling and creep of a material [2], which is a critical concern for the stability and lifetime of materials used in a nuclear reactor.

To date, the formation mechanisms of voids and dislocation loops in many irradiated materials have been extensively studied from both experimental and theoretical aspects [3,4,5,6,7]. The dependences of void and dislocation loop formations on the pre-irradiated microstructure, impurities, temperature and irradiation dose have been appropriately considered. Multiscale modeling is used to unveil the underlying mechanism of irradiation damage effects in a hierarchical manner. Phase-field model and rate theory are two typical mesoscale methods to simulate defects production, accumulation, recombination and annihilation during irradiation [8,9,10,11,12,13]. The phase-field method is able to predict microstructure evolution using a set of order parameters based on the principle of total Gibbs free energy minimization following the Cahn-Hilliard and time-dependent Ginsburg-Landau equations [14]. To describe the evolution of microstructure in terms of chemical rate processes, the mean-field rate theory has been used to calculate the reaction rates of point defects with other defects and extended sinks on average over the material [15].

In the early stage of irradiation, vacancies are difficult to aggregate into clusters, while interstitials are more likely to form clusters. This is due mainly to the distinct difference in their mobilities, for example, the vacancy mobility is ~1.64 jumps per second while interstitial mobility is $\sim 2.57 \times 10^3$ jumps per second in the neutron irradiated iron at 473 K [16]. Given this fact, it is difficult to capture the formation of voids and dislocation loops simultaneously within the phase-field method. Pervious phase-field simulation studies focused on the evolution of voids/bubbles [9,10,17,18,19] and dislocation loops [20,21,22] separately. Mean-field rate theory is commonly used to explore the evolution of defect clusters [8,11,13,23,24,25] at the same time.

In this study, we investigate the effects of temperature and irradiation dose on the evolution of irradiation-induced voids and interstitial-type dislocation loops by imposing the temperature-dependent material parameters. The radii of voids are simulated using the phase-field model and rate theory, respectively, under the same irradiation condition. The evolution of dislocation loops are investigated by the rate equations. Mesoscale simulations are performed on bcc iron and vanadium. These two metals are the major components of ferritic/martensitic steels and vanadium alloys (e.g., V-Ti-Cr alloys), respectively, which are the candidate materials for the first wall and blanket

* Corresponding author.
E-mail address: zhaojj@dlut.edu.cn (J. Zhao).

https://doi.org/10.1016/j.fusengdes.2018.10.011
Received 25 May 2018; Received in revised form 9 October 2018; Accepted 9 October 2018

structures of fusion reactor due to their good mechanical properties and high irradiation resistance [26,27]. From the simulation results, we find that voids and dislocation loops are more likely to form in vanadium than in iron. Furthermore, the increase in yield strength due to irradiation-induced defect clusters is evaluated.

2. Methods

2.1. Phase-field model for void formation

Two phases (void and matrix) and two components (vacancy (v) and self-interstitial (i)) are considered in the current phase-field model. The vacancy concentration c_v and interstitial concentration c_i are conserved fields, and the order parameter η is a non-conserved field that distinguishes the structural difference between void ($\eta = 1$) and matrix ($\eta = 0$) phases, which changes continuously from 1 to 0 across interfaces between void and matrix. The total free energy of such a system is given by

$$F = N\int ((1 - h(\eta))f^{matrix}(c_v, c_i) + h(\eta)f^{void}(c_v, c_i) + \omega_o g(c_v, c_i, \eta) + \kappa_v |\nabla c_v|^2 + \kappa_i |\nabla c_i|^2 + \kappa_\eta |\nabla \eta|^2)dV \quad (1)$$

where N is the number of lattice sites per unit volume of a material, f^{matrix} is the free energy of the matrix phase, f^{void} is the free energy of the void phase, h is an interpolation function to connect two free energy curves as function of concentrations only in the dimension of the order parameter η, g is the double-well potential, ω_o is the barrier height of the double-well potential, and κ is the gradient energy coefficient.

The free energy of the matrix phase (f^{matrix}), including the enthalpy and entropy contributions of vacancy and interstitial in the matrix phase, is expressed as [28]

$$f^{matrix} = (c_v - c_v^{eq})(E_v^f - TS_v^f) + (c_i - c_i^{eq})(E_i^f - TS_i^f) + k_B T((1 - c_v - c_i)\ln(1 - c_v - c_i) - (1 - c_v^{eq} - c_i^{eq})\ln(1 - c_v^{eq} - c_i^{eq}) + c_v \ln c_v - c_v^{eq} \ln c_v^{eq} + c_i \ln c_i - c_i^{eq} \ln c_i^{eq}) \quad (2)$$

where c^{eq} is the equilibrium concentration of vacancy or interstitial, E^f is the formation energy of vacancy or interstitial, S^f is the formation entropy of vacancy or interstitial, k_B is the Boltzmann constant, and T is the absolute temperature. The free energy of the void phase (f^{void}) is related to vacancy and interstitial concentrations

$$f^{void}(c_v, c_i) = k_B T((c_v - 1)^2 + c_i^2) \quad (3)$$

Void phase can be considered as consisting of 100% vacancies (i.e., $c_v = 1$ and $c_i = 0$). This formulism describes the growth of a vacancy cluster by absorbing vacancies and the shrinkage of a void by emitting vacancies or absorbing interstitials from the surrounding matrix. In addition, it ensures the minimum free energy of void phase ($f^{void} = 0$) is in the case of $c_v = 1$ and $c_i = 0$. The coefficient $k_B T$ in Eq.(3) is used to normalize the free energy of void phase in the following calculations [29]. The function $h(\eta) = \eta^3(6\eta^2 - 15\eta + 10)$ is frequently used to interpolate the interface between the matrix and void phases. The double-well potential (g), which represents the energy barrier at the matrix/void interface, adopts the following form [28]

$$g(c_v, c_i, \eta) = B_1(c_v - 1)^2\eta^2 + B_2(\eta - 1)^2(c_v - c_v^{eq})^2 + B_3 c_i^2\eta^2 + B_4(\eta - 1)^2(c_i - c_i^{eq})^2 + B_5(c_v - 1)^2(c_i - c_i^{eq})^2 + B_6(c_v - c_v^{eq})^2 c_i^{eq} \quad (4)$$

where B_1 to B_6 are constants and set as 1.0.

The time-evolution of two conserved fields, c_v and c_i, and the non-conserved field, η, are described by the Cahn-Hilliard nonlinear diffusion equation and the time-dependent Ginsburg-Landau (or Allen-Cahn) equation, respectively. Since the point defects (i.e., vacancies and self-interstitials) are produced during irradiation and their interaction can affect the evolution of the conserved field, a production term P and a recombination term R_{iv} are added in the conserved fields. In addition, the structural defects in materials, such as grain boundaries and dislocations, are the sinks for vacancies and self-interstitials, which can influence the evolution of defect clusters. The point defect concentration fields and the evolution of the order parameter are constructed as

$$\frac{\partial c_v}{\partial t} = \nabla\left(M_v \nabla \frac{1}{N}\frac{\delta F}{\delta c_v}\right) + \xi_v + P_v - R_{iv} - R_v^{sink} \quad (5)$$

$$\frac{\partial c_i}{\partial t} = \nabla\left(M_i \nabla \frac{1}{N}\frac{\delta F}{\delta c_i}\right) + \xi_i + P_i - R_{iv} - R_i^{sink} \quad (6)$$

$$\frac{\partial \eta}{\partial t} = -L\frac{\delta F}{\delta \eta} + \xi \quad (7)$$

where M is the mobility of a given type of point defect and is expressed as $M = Dc/k_B T$, D is the diffusivity, L is the mobility of void surface, R^{sink} is the sink term, and ξ is the Langevin noise terms characterizing thermal fluctuations in the composition and structural order parameter, respectively. Usually, the Langevin noise term follows the normal distribution and they are switched off at some later time when enough nuclei have been generated. To ensure void nucleation to take place during a stochastic process, small integration time steps and fine length scales are required to capture the void formation phenomena using Langevin equation in a quantitative way [30].

The spatial distribution of defects shows a vacancy cluster at the center of cascade and an interstitial rich out-shell during the displacement cascade. Large fractions of Frenkel pairs recombine within the cascade core. From molecular dynamics simulations, Stoller [31] found that the surviving fractions of interstitials and vacancies vary from ~1.0 at low cascade energy to ~0.3 for high cascade energy greater than 10 keV under neutron energy spectrum. In our phase-field model, the vacancy source term P_v and the self-interstitial source term P_i are related to the irradiation condition. For example, if the order parameter η is less than 0.8 and the random number Ran is less equal than the probability of a cascade occurring within a volume per time (P_{casc} in unit of dpa/s), the production of point defects can be expressed as $P_v = 1/BP_i = P_{casc}V_G$. Here V_G is the maximum increase in vacancy (or interstitial) concentration due to irradiation [32] and $V_G = 1$ is used in the simulations to ensure the increment of defects concentrations, and B is a bias between vacancy and interstitial production efficiencies in the cascade, which is highly sensitive to the void growth rate [33]. Based on the production bias model, the difference in the stability and lifetime between vacancy and interstitial clusters produced during the cascade process shows an asymmetric production in the amounts of vacancies and interstitials [33,34]. This production bias is considered as a potent driving force for void growth under the cascade damage condition. In the current phase-field model of irradiation-induced void, a bias B in $P_i = BP_v$ is chosen to mimic the dislocation bias that the self-interstitial atoms prefer to being absorbed at the dislocation, leading to vacancy accumulation and void formation. Millett et al. suggested a production bias of 0.9 by creating 10% more vacancies inside the system, which is able to mimic a dislocation bias [10].

Vacancies and self-interstitials diffuse randomly through the lattice and combine with each other to annihilate. The recombination term in Eqs.(5)–(6) is given by $R_{iv} = R_r c_v c_i$, which mimics the recombination expression in the rate theory [35]. It should be pointed out that in addition to the vacancy-interstitial recombination in the matrix, the interstitial atom arriving at the void/matrix interface will lose its identity and the corresponding mutual recombination may differ from that in the matrix. According to Ref. [10], a rate parameter R_r dependent on both bulk and surface terms is considered as $R_r = R^{bulk} + \eta^2 R^{surf}$. In this case, the structural order parameter η allows us to consider the recombination process that occurs in either matrix or void. The vacancy and interstitial annihilation at sinks can be described by $R_n^{sink} = k_n^2 D_n(c_n - c_n^{eq})$ with $n = v, i$, where k_n^2 is the total sink strength of structural defects (e.g., grain boundary and dislocation) for