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A phase field modeling based study of microstructure evolution and its influence on thermal conductivity in polycrystalline tungsten under irradiation

Hao Wang[a], Sudipta Biswas[a], Yousung Han[b], Vikas Tomar[a,*]

[a] School of Aeronautics and Astronautics, Purdue University, West Lafayette, IN 47907, USA
[b] Department of Mechatronics Engineering, Incheon National University, Yeonsu-gu, Incheon 22012, South Korea

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ABSTRACT

In this work, we study effects of neutron irradiation and elastic tensile loading on microstructure evolution in polycrystalline tungsten by using a phase field modeling based approach. The proposed model involves the interaction of point defects with grain boundaries (GBs), thermal resistance of GBs, and voids. The void evolution analysis shows that the elastic energy field affects the shape and growth rate of voids. The overall trend of porosity evolution during irradiation follows the Johnson-Mehl-Avrami-Kolmogorov (JMAK) equation. Voids nucleation and growth can reduce both elastic strain energy and chemical free energy in the system. In addition, increase of porosity could significantly degrade the effective thermal conductivity of analyzed tungsten polycrystalline microstructures. The observations comply with the predictions from the theoretical models.

1. Introduction

Tungsten (W) is one of the primary candidate materials for structural components of nuclear fusion reactors due to its excellent high temperature thermal and mechanical properties. It has high melting point (T_m = 3695 K), high thermal conductivity, and high sputtering resistance. Structural components such as first wall and diverter for the next generation nuclear fusion reactors are exposed to high levels of neutron radiation and irradiation damage up to 120 dpa (displacements per atom) [1]. Such high levels of irradiation may lead to microstructural changes and deterioration of material properties mostly due to void-induced swelling. The nucleation and growth of voids during irradiation has been observed in several structural materials, including face-centered cubic, body-centered cubic, and hexagonal-closed-packed materials [2–7]. The volume fraction, morphology, and kinetics of voids significantly affect material properties, such as tensile strength, creep strength, and thermal conductivity [8,9]. Recently researchers have also focused on developing materials tolerant of radiation damages [10]. Understanding the irradiation induced damage behavior and its impact on the material properties will contribute to the advancements in the field of nuclear materials. Therefore, it is very important to understand and predict the evolution of the microstructural features under irradiation and their impact on physical properties.

Microstructural evolution of nuclear materials is a complex multi-scale and multi-physics phenomenon consisting of many interacting and competing mechanisms, including radiation-induced defects formation, gas bubbles creation, grain boundary (GB) migration, grain growth etc. A range of experimental measurements on polycrystalline tungsten have been performed to study microstructural evolution under irradiation. Among such researches, Iwakiri et al. [11] performed transmission electron microscopy (TEM) analyses to examine the temperature effect on the growth rates of dislocation loops and Helium bubbles irradiated by 8 and 0.25 keV H+ ions. The changes in microstructure and irradiation hardening under the influence of transmutation elements such as rhenium (Re) and osmium(Os) due to high-energy neutron exposure was also studied in the temperature range of 400–750 °C [12]. Despite experimental measurements, the exact science of microstructure evolution as a function of radiation fluence remains unclear. This issue is complicated by the fact that it is not only challenging but also costly to perform irradiation experiments with realistic levels of irradiation energy and irradiation exposure time to understand microstructure evolution [13]. For this reason, most studies do not analyze the exact same microstructure at different irradiation fluences. Modeling and simulation based studies can significantly contribute to understanding the science of microstructure evolution under irradiation. Different modeling approaches used for predicting microstructural changes are classical molecular dynamics (MD), *ab-initio* calculations using density function theory (DFT), kinetic Monte Carlo

* Corresponding author.
E-mail address: tomar@purdue.edu (V. Tomar).

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(KMC) and dislocation dynamics (DD) [14]. Each of these methods are valid for a particular time and length scale and have their own limitations. In the present work, phase field modeling (PFM) is adopted for capturing the effect of irradiation on the morphological changes in microstructural features as well as on material property degradation. Being a mesoscale modeling approach, PFM helps in quantifying the impact of microstructural changes on the bulk properties of materials.

The PFM has been used to study phase transformation and kinetics of microstructure evolution in a variety of materials and processes, including solidification [15,16], solid-state phase transformations [7,17,18], grain growth [19], solute-dislocation interactions [20], and crack propagation [21]. In PFM, microstructural features are represented by phase-field variables having specific equilibrium values corresponding to each constituent phase. The PFM uses thermodynamic free energy values obtained from atomistic simulations, thermodynamic calculations, or experiments [22]. The phase-field variables evolve in space and time such that the total free energy of the analyzed material system reduces. There are two types of phase-field variables considered in this approach: the first type being the concentration field variable which represents conserved features such as composition, density etc. and the other being the order parameter illustrating the non-conserved micro-structural features such as grain orientation, void fraction etc. The microstructural evolution is governed by the Cahn-Hilliard (CH) diffusion equation for conserved variables [23] and Allen-Cahn (AC) equation for non-conserved variables. PFM has been used to study changes in microstructural features under irradiation, such as nucleation and growth of gas bubbles and voids, and the evolution of overall precipitate morphology. In the current work, the primary focus is on capturing the microstructural changes based on void formation and void clustering during irradiation and relating such changes to microstructure change dependent thermal conductivity calculations.

2. Computational details

In this work, the analyzed material microstructure is considered to have two distinct equilibrium phases: one is the matrix phase with point defects, such as vacancies and interstitials, and the other one is the void phase. Distribution of vacancies and interstitials in the matrix phase are represented by the corresponding concentration field variables denoted by $c_v(r,t)$ and $c_i(r,t)$, respectively. The initial point defect concentrations in the matrix are assumed to be at a super saturation level to accelerate the void nucleation and void growth processes. Voids are formed due to accumulation of vacancies. Thus the void phase can be treated as having 100% vacancy concentration (i.e. $c_v = 1$). A non-conserved order parameter $\eta(r,t)$ is used to identify different phases, which takes a value of one inside the void phase and zero within the matrix phase, with linear variation across the matrix-void interface. Vacancy and interstitial concentration fields and the order parameter are assumed to have both spatial and temporal continuities.

In PFM, the total free energy of the system is represented as a combination of bulk free energy, elastic strain energy and interfacial free energy of the constituent phases. Following the Cahn-Hilliard [24] definition of the free energy for a non-equilibrium multiphase system, the total free energy, F, of a system is expressed using the vacancy concentration $c_v(r,t)$, interstitial concentration $c_i(r,t)$, and order parameter $\eta(r,t)$, as

$$F(c_v,c_i,\eta,T) = \int \left[f_0(c_v,c_i,\eta,T) + f_{el}(c_v,c_i,\eta) + \frac{\kappa_v}{2}|\nabla c_v|^2 + \frac{\kappa_i}{2}|\nabla c_i|^2 + \frac{\kappa_\eta}{2}|\nabla \eta|^2 \right] dV, \tag{1}$$

where $f_0(c_v,c_i,\eta,T)$ is the combined chemical free energy density function, including both matrix and void phases, $f_{el}(c_v,c_i,\eta)$ represents elastic strain energy, and all the other gradient terms represent the interfacial free energy.

2.1. Chemical free energy density

Based on the work of Millett et al. [25] and Rokkam et al. [26], the chemical free energy density used for a binary material system consisting of matrix and void phases is represented as

$$f_0(c_v,c_i,\eta,T) = h(\eta)\psi(c_v,c_i,T) + \omega(c_v,c_i,\eta), \tag{2}$$

where $h(\eta)$ is the shape function, $\psi(c_v,c_i,\eta,T)$ is the defect free energy density term, and $\omega(c_v,c_i,\eta)$ is a Landau-type term. The defect free energy density term, $\psi(c_v,c_i,T)$, is derived in terms of the enthalpic and entropic contributions of vacancies and interstitials, and it is written as

$$\psi(c_v,c_i,T) = (E_v^f c_v + E_i^f c_i + K_B T(c_v \log(c_v) + (1-c_v)\log(1-c_v) + c_i \log(c_i) + (1-c_i)\log(1-c_i))), \tag{3}$$

where E_v^f is the vacancy formation energy, E_i^f is the interstitial formation energy, K_B is the Boltzmann constant, and T is the absolute temperature value in Kelvin. The shape function is considered as $h(\eta) = (\eta-1)^2(\eta+1)^2$, which ensures the entropy term contributes towards evolution of the point defects concentration only within the matrix phase and not within the void phase. The Landau-type term $\omega(c_v,c_i,\eta)$ is responsible for bi-stability in the system, formulated as [26]

$$\omega(c_v,c_i,\eta) = -A((c_v-c_v^0)^2 + (c_i-c_i^0)^2)(\eta^4-3\eta^2+2\eta) + B((c_v-1)^2 + c_i(2-c_i))\eta^2, \tag{4}$$

where c_v^0 and c_i^0 are the equilibrium concentration of vacancies and interstitials in the matrix respectively, and A and B are constant prefactors related to the material. The equilibrium concentration values

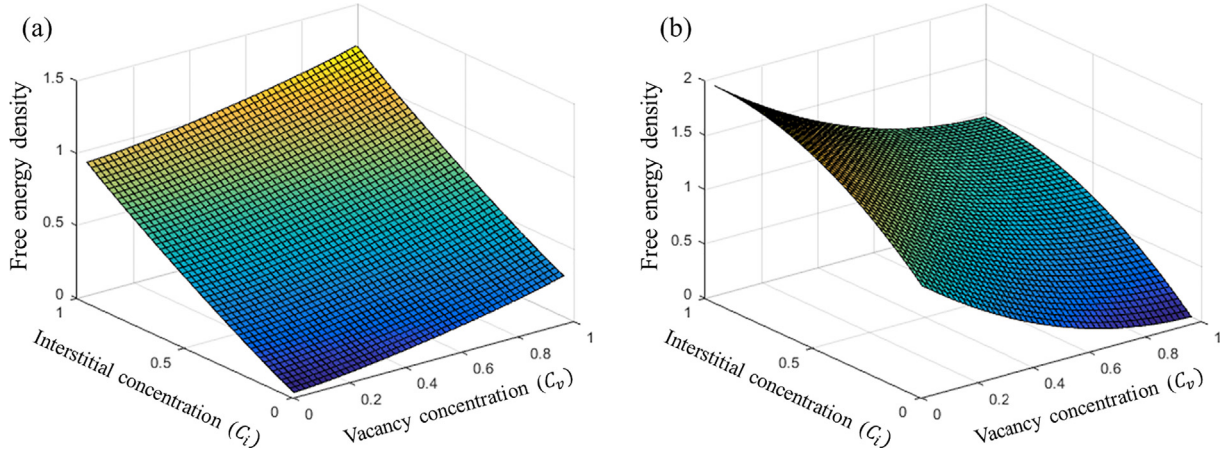

Fig. 1. Free energy density distribution (a) matrix phase; (b) void phase.