A phase field study of microstructure evolution of polycrystalline tungsten under irradiation

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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. The volume fraction, morphology, and kinetics of voids significantly affect material properties, such as tensile strength, creep strength, and thermal conductivity [1,2]. 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. 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.

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. Details on chemical free energy, elastic energy, and their numerical implementation are available in author's previous work [3].

3. Results

Fig. 1 shows temporal evolution of vacancy concentration map in the polycrystalline tungsten at 1000K under a neutron flux value of 2 x 10^{18} n/cm^2·s. Polycrystalline microstructures are generated using Voronoi tessellation method. Voids nucleation in a single crystalline structure with an initial supersaturated point defect concentration is considered for preliminary examination of the point defect source term. As observed in Fig. 1, neutron impact positions are located randomly in the matrix phase and local vacancy concentration increases due to the cascade effect. After a period of time, adjacent vacancies interact with each other and aggregate into vacancy clusters. When a cluster of vacancies exceeds certain concentration value, it could form a stable phase, considered as a void. Eventually, the irradiation process causes the morphology of voids to change from round to an oval shape as the vacancy clusters accumulate leading to formation of new voids. Once a void phase is formed, free energy function drives the local interstitial concentration to decrease inside the void, reaching zero. Therefore, comparing to the matrix phase, the void phase has much lower interstitial concentration. As flux increases, frequency of neutron collisions also increases, which impacts the point defect generation rate. Thereafter, rate of porosity evolution is higher with higher flux. The porosity evolution trend follows the Johnson-Mehl-Avrami-Kolmogorov (JMAK) equation [4-6], expressed as

$$X(t) = 1 - \exp(-kt^m). \quad (1)$$

Here, X(t) is the volume fraction of the newly transformed phase, k is the characteristic constant of nucleation kinetics in the system, and m is an exponent which characterizes the degree of heterogeneity of the analyzed system. The JMAK equation has the S-curve form: i.e., the nucleation rate first accelerates and then decelerates. This is mainly due to the surface energy and the chemical potential energy difference between solid and vacancy phases, which yields an energy barrier for void nucleation. Local vacancy clusters have to grow large enough to overcome the free energy barrier for voids nucleation

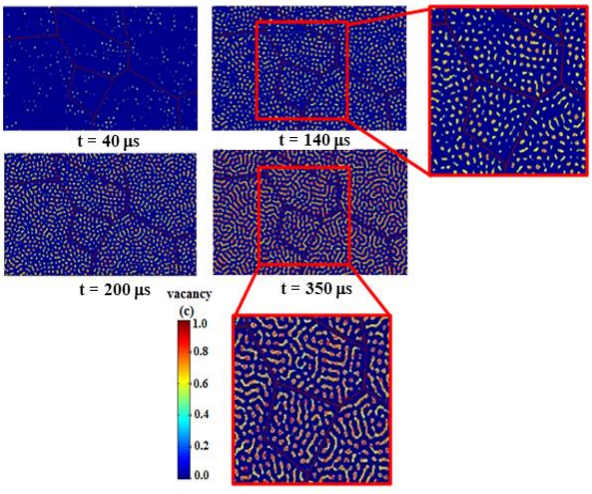

Fig. 1. Void nucleation in poly-crystalline structure (average grain size 1.5μm) under irradiation at 1000K. Time increases from left to right as, 40μs, 140μs, 200μs and 350μs.

Within the grain interiors, the voids exhibit similar behavior as the single crystalline case discussed earlier. However, due to the presence of GBs, the overall evolution process varies. The solid blue lines exhibit the position of GBs in the microstructure, which also indicates zones with low point defect concentrations. This is due to the annihilation effect of GBs. They act as an efficient sink for irradiation-induced point defects and defect clusters, and create a point defects free zone nearby. In these regions, vacancy concentration will never surpasses the critical value for stabilized void embryos, thereby, these regions are also known as void denuded zone.

3. Conclusions

In the present study, a phase field model is proposed based on the work of Millett et al. [7] and Rokkam et al. [8] to predict microstructure evolution in polycrystalline tungsten. The model is extended to include elastic tensile loading along with neutron irradiation, to study how the elastic energy field affects void nucleation and evolution in polycrystalline tungsten. Both vacancy and interstitial are considered in current model. The void evolution analysis shows that the elastic energy field could strongly affect the shape and growth rate of voids. Both elastic energy and chemical free energy affect porosity evolution. Simulation results in polycrystalline tungsten exhibit that the current phase-filed model captures the void nucleation and its interaction with the GBs leading to creation of a point defect free zone in the vicinity of GBs. It also involves thermal resistance of GBs and gas bubbles, and captures how effective thermal conductivity degrades as a function of porosity and average grain size. The results correlate well with theoretical model predictions.

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