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Asymptotic and uncertainty analyses of a phase field model for void formation under irradiation

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ABSTRACT

We perform asymptotic analysis and uncertainty quantification of a phase field model for void formation and evolution in materials subject to irradiation. The parameters of the phase field model are obtained in terms of the underlying material specific quantities by matching the sharp interface limit of the phase field model with the corresponding sharp interface theory for void growth. To evaluate the sensitivity of phase field simulations to uncertainties in input parameters we quantify the predictions using the stochastic collocation method. Uncertainties arising from material parameters are investigated based on available experimental and atomic scale data. The results of our analysis suggest that the uncertainty in the formation and migration energies of vacancies are found to have a strong influence on the void volume fraction (or porosity). In contrast, the uncertainty resulting from the void surface energy has minimal affect. The analysis also shows that the model is consistent in the sense that its predictions do not drastically change as a result of small variations of the model input parameters.

1. Introduction

Phase field modeling of microstructure evolution is becoming important in studying radiation effects in materials; see [1–8] for phase field models of void formation and growth. The phase field approach has been brought into this area following its successful application to many materials science problems involving diffusion processes and interfacial motion [9,10]. An advantage this approach offers is the ability to resolve spatial realizations of the evolving microstructure and consequently it has the potential to reveal the synergistic aspects of defect and microstructure dynamics in irradiated solids. A phase field model for void formation in irradiated solids has been recently developed by merging defects diffusion and interface evolution into a type C framework [11] that combines both Cahn–Hilliard and Allen–Cahn dynamics [1–5]. The model reproduces several important microstructural characteristics of void dynamics under irradiation, e.g., nucleation, void growth and domain swelling, through qualitative simulations. However, its application to model real engineering materials has been limited due to lack of material specific phase field model parameters. The phase field models can be theoretically connected to their equivalent sharp interface models – free boundary problem which is usually cast in the form of measurable quantities – using formal asymptotic analysis [12–14]. To perform quantitative modeling of voids in specific materials, it is required to verify the consistency of the phase field model for void formation and map the model parameters to corresponding sharp interface quantities using the asymptotic matching techniques. The resulting model parameters can be determined directly from material specific physical quantities which can be obtained via experiments or from lower scale atomistic models. While simulations based on phase field models provide a powerful tool to understand the complex phenomenon of irradiation induced microstructural changes (like void formation), it is essential to evaluate their reliability as a function of certainty in input parameters. The systematic underpinning of the phase field model parameters and quantification of the model predictions based on input parameter uncertainties is of huge interest for the development of next generation mesoscopically informed material response codes. We address both these aspects for the process of interest – void evolution under irradiation, using a phase field model for void formation under irradiation as starting point.

In this communication we perform asymptotic analysis of a class of phase field models of type C that have been recently used to model void formation under irradiation [1,5] and fix the phase field model parameters in terms of conventional properties of the solid material of interest. We then systematically evaluate the sensitivity of the void formation predictions in response to

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input material parameter uncertainties using a stochastic collocation based uncertainty quantification (UQ) method. The model prediction is quantified using the average void volume fraction in the solid under irradiation. Multiple simulations of the void evolution process are performed with material parameters input sampled from physical parameter distributions and adequate statistics are gathered to determine the average void volume fraction and its standard deviation.

The paper is organized as follows: in Section 2 we first give a brief description of the phase field model for void evolution under irradiation and then discuss the asymptotic analysis performed to connect the phase field model parameters with materials parameters. Subsequently, we identify the uncertainty in material parameters based on relevant data from literature. In Section 3, we introduce the UQ methodology and the simulation framework used in this study. In Section 4, we discuss the numerical simulation results and summarize our work in Section 5.

2. Phase field model for void evolution under irradiation

Over the past fifteen years or so, the phase-field method has emerged as a powerful computational approach to solving interfacial dynamics problems [10,15–18]. The popularity of this method comes from its efficiency in dealing with the generally time-consuming interface motion calculations in two and three dimensions. The use of an order parameter as a diffuse representation of the interface helps to reduce the problem of interface motion into one for the time evolution of the order parameter and hence greatly alleviates the computation required in classic sharp-interface description. The phase field model we discuss in this work has been used to model void formation in irradiated materials. The void nucleation rate calculated from this model has the same behavior as predicted by Kolmogorov–Johnson–Mehl–Avrami (KJMA) theory, while the post-nucleation growth is governed by an Ostwald ripening process [1,5]. In the presence of microstructural features like grain-boundaries, a void denuded zone can be identified near the grain-boundary along with void occupied inner grain region [2,5], which is commonly observed in experiments.

2.1. Phase field model formulation

The phase-field model for irradiation induced void formation of interest to us is an extension of the one developed by Rokkam and co-workers [1–5]. A summary of the phase-field model used for the current work is summarized in this sub-section. For more details on model the reader is referred to [5]. The model describes the free energy of a metal comprising of two distinct phases: a matrix phase with point defect concentrations near thermodynamic equilibrium and a void phase defined as a cluster of vacancies only. The free energy functional of the heterogeneous system is written in terms of its constituent phases and interfaces as,

$$F = \int N\Big[K_v|\nabla c_v|^2 + K_i|\nabla c_i|^2 + K_\eta|\nabla\eta|^2 + (1-h(\eta))f^{mat} + h(\eta)f^{void} + \omega g(c_v, c_i, \eta)\Big]dV. \tag{1}$$

The first three terms are gradient contributions due to vacancy concentration, c_v, interstitial concentration, c_i, and order parameter, η, with their respective gradient coefficients, K_v, K_i, and K_η. The bulk matrix free energy f^{mat} is

$$\begin{aligned} f^{mat} = {} & (c_v - c_v^0)\left(E_v^f - Ts_v^f\right) + (c_i - c_i^0)\left(E_i^f - Ts_i^f\right) \\ & + k_B T[(1-c_v-c_i)\ln(1-c_v-c_i) \\ & - (1-c_v^0-c_i^0)\ln(1-c_v^0-c_i^0) + c_v \ln c_v - c_v^0 \ln c_v^0 \\ & + c_i \ln c_i - c_i^0 \ln c_i^0], \end{aligned} \tag{2}$$

with thermal equilibrium concentration of vacancy c_v^0 and interstitial c_i^0, defect formation energy of vacancy E_v^f and interstitial E_i^f, temperature T, entropy of defects s_v^f (vacancy) and s_i^f (interstitial), and Boltzmann constant k_B. The interpolation function $h(\eta)$ used to interpolate over the interface between the matrix and void phases has the form,

$$h(\eta) = \eta^3(6\eta^2 - 15\eta + 10). \tag{3}$$

In the last term, ω is a pre-factor and $g(c_v, c_i, \eta)$ is a Landau polynomial which has the following form

$$\begin{aligned} g(c_v, c_i, \eta) = {} & \Big[B_1(c_v-1)^2\eta^2 + B_2(\eta-1)^2\left(c_v-c_v^0\right)^2 + B_3 c_i^2\eta^2 \\ & + B_4(\eta-1)^2\left(c_i-c_i^0\right)^2 + B_5(c_v-1)^2\left(c_i-c_i^0\right)^2 \\ & + B_6\left(c_v-c_v^0\right)c_i^0\Big], \end{aligned} \tag{4}$$

with dimensionless constants B_1 through B_6. For more details on the construction and nature of $g(c_v, c_i, \eta)$ please refer [5]. All terms within the integrand of Eq. (1) have a dimension of energy per lattice site. With the factor N, the number of sites per unit volume in front, the volume integral gives the total free energy in the system. A thermodynamically consistent phase field model for void evolution under irradiation [5] is given by a set of equations describing the evolution of the vacancy, interstitial and order parameter fields:

$$\frac{\partial c_v}{\partial t} = \nabla\cdot\left(M_v\nabla\frac{1}{N}\frac{\delta F}{\delta c_v}\right) + \zeta_v + P_v^{casc} - R_{vi} - R_v^{sink}, \tag{5}$$

$$\frac{\partial c_i}{\partial t} = \nabla\cdot\left(M_i\nabla\frac{1}{N}\frac{\delta F}{\delta c_i}\right) + \zeta_i + P_i^{casc} - R_{vi} - R_i^{sink}, \tag{6}$$

$$-\frac{\partial\eta}{\partial t} = L_\eta\left(\frac{\delta F}{\delta\eta}\right) + \zeta_\eta, \tag{7}$$

In the above, M_v, M_i, and L_η are the kinetic coefficient or mobilities associated with the evolution equations; ζ_v, ζ_i and ζ_η are thermal noise terms; P_v^{casc} and P_i^{casc} are source terms corresponding to stochastic generation vacancies and interstitials as a function of irradiation. R_{vi} is the vacancy-interstitial reaction rate and R_v^{sink}, R_i^{sink} are microstructural sinks for point defects. The functional derivatives $\frac{\delta F}{\delta c_v}$, $\frac{\delta F}{\delta c_i}$ and $\frac{\delta F}{\delta\eta}$ are given by

$$\frac{1}{N}\frac{\delta F}{\delta c_v} = (1-h(\eta))f_v + \omega\frac{\partial g(c_v, c_i, \eta)}{\partial c_v} - 2K_v\nabla^2 c_v, \tag{8}$$

$$\frac{1}{N}\frac{\delta F}{\delta c_i} = (1-h(\eta))f_i + \omega\frac{\partial g(c_v, c_i, \eta)}{\partial c_i} - 2K_i\nabla^2 c_i, \tag{9}$$

$$\frac{1}{N}\frac{\delta F}{\delta\eta} = \omega\left[-h'(\eta)\frac{f^{mat}}{\omega} + h'(\eta)\frac{f^{void}}{\omega} + \frac{\partial g(c_v, c_i, \eta)}{\partial\eta}\right] - 2K_\eta\nabla^2\eta, \tag{10}$$

with

$$f_v = \left(E_v^f - Ts_v^f\right) + k_B T\ln\left(\frac{c_v}{1-c_v-c_i}\right), \text{and}$$

$$f_i = \left(E_i^f - Ts_i^f\right) + k_B T\ln\left(\frac{c_i}{1-c_v-c_i}\right).$$

Since the dependence of functions $h(\eta)$ and $g(c_v, c_i, \eta)$ on the respective field variables is implicit, for brevity of the equations we will use $h(\eta) \equiv h$ and $g(c_v, c_i, \eta) \equiv g$ in subsequent sections. Likewise, the energy terms will be denoted using $f^{mat} \equiv f$ and $f^{void} \equiv \tilde{f}$.

As demonstrated in previous works, this model is capable of producing void nucleation and growth for material under irradiation by treating void as a space filled only by vacancies, see [1–5]. Among many interesting simulation results, the evolution of void volume fraction in the solid is one of the most important aspects of the microstructure change under irradiation (Fig. 1). Porosity P can be defined as the volume fraction of void phase