Current Opinion in Solid State and Materials Science 18 (2014) 90–98

Contents lists available at ScienceDirect

Current Opinion in Solid State and Materials Science

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

Diffuse interface modeling of void growth in irradiated materials. Mathematical, thermodynamic and atomistic perspectives

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ARTICLE INFO

Article history:
Received 22 August 2013
Revised 23 October 2013
Accepted 4 January 2014
Available online 30 January 2014

Keywords:
Void growth
Irradiated materials
Phase field model
Radiation effects
Sharp interface model

ABSTRACT

We present an assessment of the diffuse interface models of void growth in irradiated materials. Since the void surface is inherently sharp, diffuse interface models for void growth must be constructed in a way to make them consistent with the sharp-interface description of the problem. Therefore, we first present the sharp-interface description of the void growth problem and deduce the equation of motion for the void surface. We also compare two existing phase field models to determine which one corresponds to the sharp-interface analysis. It was shown that a phase field model of type C, which couples Cahn–Hilliard and Allen–Cahn equations, is the most adequate since this type of model can take into account the reaction of point defects at the void surface via an Allen–Cahn equation. Fixing the model parameters in the diffuse interface model is discussed from the points of view of asymptotic matching. Sample results for void growth in a single component metal based on sharp and diffuse interface models are presented. Finally, a perspective on the use of atomistic modeling in both constitutive and nucleation modeling within the phase field approach for void formation in irradiated materials is presented.

1. Introduction

Neutron irradiation affects the performance and lifetime of nuclear reactor components. Such a kind irradiation produces large densities of vacancies and interstitials, the diffusion and clustering of which result in the formation of microstructural features such as dislocation loops and voids in irradiated materials [1,2]. These microstructural features influence the dimensional stability and mechanical properties of materials [3,4]. Voids are particularly important since their presence leads to swelling [5]. Theoretical models were proposed to investigate void formation and growth in irradiated materials [6–14]. These models fall into three categories. The first includes clustering and nucleation type models [6–8], which are concerned with void nucleation as a result of localized fluctuations in the vacancy concentration. A characteristic feature of these models is the existence of a nucleation barrier that must be overcome in order for void nucleation to take place. The second category includes models for void lattice formation [9–11]. Spinodal instabilities of homogeneous vacancy concentrations, elastic interaction of voids and reaction–diffusion aspects of point defects were suggested as possible ordering mechanisms. The last category includes void growth models based on the chemical reaction rate theory [12–14]. This theory considers the point defect and sink concentrations to be spatially uniform fields influencing the growth of a representative void. A typical rate theory model consists of three equations for the rate of change of vacancy and interstitial concentrations and void radius [1,2]:

$$\dot{c}_v = P_v - K_{vi}c_v c_i - K_{vs}c_v c_s, \tag{1a}$$

$$\dot{c}_i = P_i - K_{vi}c_v c_i - K_{is}c_i c_s, \tag{1b}$$

$$\dot{R} = [D_v(c_v - c_v^{eq}) - D_i(c_i - c_i^{eq})]\Omega/R. \tag{1c}$$

In the above, c_v and c_i are the average vacancy and interstitial concentrations in the irradiated solid, P_i and P_v are the respective production terms, K_{vi} is a rate constant for vacancy–interstitial recombination, K_{vs} and K_{is} are rate constants for defects reaction with sinks of average concentration c_s, R is the void radius, Ω is the atomic volume, c_v^{eq} and c_i^{eq} are the equilibrium vacancy and interstitial concentrations at the void surface, and D_v and D_i are the diffusion coefficients of vacancies and interstitials, respectively.

It is noted that Eq. (1c) for the void growth rate is practically the same as the rate equation for diffusion-controlled precipitate growth from supersaturated matrix in the classical Lifshitz–Sly-

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http://dx.doi.org/10.1016/j.cossms.2014.01.002
1359-0286/

ozov–Wagner theory [15,16] and the Mullins–Sekerka quasistatic models [17]. This similarity stems from the fact that the rate theory assumes that the point defect concentrations at the void surface take on their thermal equilibrium values and hence the growth process is completely controlled by the diffusion of point defects from the bulk to the void surface. The process of void growth, however, is not necessarily diffusion-controlled and the reaction of point defects at the void surface must be taken into consideration in determining the rate of the growth process [18]. The idea of considering the reaction of defects with voids surface was discussed a while back [19,20], although this was later discarded. An important part of the current work is to show that, as a thermodynamic requirement, reactions of point defect with the void surface must be considered in the treatment of non-equilibrium void growth. This theoretical proof does not, however, aim to prove that void growth is diffusion- or reaction-controlled in the sense these terms are used in the literature [21], but it is rather a statement that reaction of defects at the void surface must be considered in defining the boundary conditions for the diffusion of defects in the solid around the voids. As explained later, this has important implications as to how diffuse interface (phase field) models for voids growth should be constructed.

Unlike nucleation from a supersaturated state or growth in a uniform species background [21], void nucleation and growth in irradiated materials take place under a highly non-equilibrium condition involving generation, diffusion and reaction of defects. The recent surge in interest in nuclear materials performance modeling has led members of the community to adopt the concepts of phase field approach to model voids in irradiated materials [22–33]. This new modeling direction was in part motivated by the need to resolve the nucleation and growth processes in space and time, and to treat the interaction of defects and the growing features, voids in this case, with other extended defects explicitly. Phase field modeling was thus viewed as a means to resolve all temporal and spatial effects in microstructure growth under irradiation and to handle nucleation and growth concurrently.

The initial phase field modeling of voids nucleation and growth adopted a simple intuition of how defects, especially vacancies, agglomerate to form voids and how they contribute to the subsequent growth of such features. Two modeling approaches emerged. In the first approach, [23–28], the process of void formation and growth was viewed as a spinodal instability in media that are supersaturated with vacancies. As such, a generalized diffusion equation of the Cahn–Hilliard type was adequate to describe void nucleation and growth. In the second approach [29–32], both Cahn–Hilliard and Allen Cahn equations were used. Both approaches made the assumption that the void surface can be modeled as a diffuse interface. Aside from the model construction and the assumptions made therein, and further keeping the accuracy of predictions of these preliminary models aside, both kinds of models seem to capture the spatial and temporal details of void formation and evolution in materials under irradiation. A fundamental question then arises as to how such two seemingly different approaches can capture the same process and whether any of these approaches can be proved to represent the physics of the problem with a higher fidelity. A second related question is how to properly construct a phase field framework for voids and what are the steps required in this regard. These two fundamental questions are addressed in this communication.

Motivated by the above questions, we discuss void growth modeling within the phase field framework here. The discussion focuses on three issues. First is the fact that, being inherently sharp interface microstructure features in solids, voids do not naturally fit into the phase field framework. As such, phase field modeling of void evolution in irradiated solids is a matter of a mathematical choice. As discussed in Section 2, the diffuse interface formalism of inherently sharp interface problems has been a successful tradition in modeling microstructure and morphological evolution problems [34–36]. Therefore, this formalism can in principle be used to model void evolution. The second issue is that, having elected to pursue this problem within the framework of diffuse interface modeling, what modeling steps are required to ensure consistency of the void growth model? By consistency here, we mean both thermodynamic consistency and consistency with the sharp-interface formalism itself. The third issue has to do with requiring the phase field models to handle void nucleation concurrently with growth and coarsening. As is well known to experts in this modeling area, the phase field approach is a continuum mesoscale modeling apparatus that discards the discrete atomistic nature of the material and it treats interfacial dynamics in terms of capillary quantities such as surface and interface energies. While the capillary nature of voids is well acknowledged in the classical nucleation theory [21], nucleation models such as cluster dynamics is inherently based on the atomic nature of defect clusters as they are based on single-defect transitions among different cluster sizes [37]. The discrete nature of transitions from one cluster size to another is also an essential feature of simulation models such as Monte Carlo [38].

In order to address the first issue above, a quick review of phase field approach is presented in Section 2, focusing on diffuse interface representations of inherently-sharp interface problems and the analyses required to ensure consistency of these models with the corresponding sharp interface formulations. In Sections 3 and 4, we present thermodynamically based sharp and diffuse interface formulations of the void growth problem and briefly discuss the analysis required to match these formulations. In Section 5, we discuss the modeling of gradient free energy terms and nucleation mechanism within the phase field framework, along with the role of atomistic simulations in guiding such a modeling and providing the needed lower scale input. We conclude with some remarks summarizing the contributions made here.

2. Phase field formalism of sharp interface problems

Phase field modeling has been widely used in predicting microstructural evolution in materials [34–36]. The main feature of this approach is the treatment of the interfaces between phases as diffuse, while the material properties of interest, which are represented by phase fields or order parameters, are assumed to change rapidly but smoothly across the interfaces. The position of the interface is implicitly given by a constant phase field level, which obviates the necessity of explicitly tracking the interface. Based on this powerful concept, phase field methods enabled the simulation of complex evolution problems such as the solidification [39], solid-state transformations [40], grain growth [41–43], crack propagation [44], dislocation dynamics [45], sintering [46–48], electromigration [49,50] and vesicle membranes [51]. Historical developments of the diffuse interface concepts can be traced back to the works of Van der Waals on gas condensation [52], Landau on phase transitions [53] (where the concept of order parameter or phase field was first introduced), Landau and Ginzburg [54] on superconducting states [54], and Cahn and Hilliard on the thermodynamics of heterogeneous systems [55]. In all of these and in subsequent works, order parameters may represent conserved quantities such as mass and energy density or non-conserved quantities such as polarization, long-range order and grain orientation. In analogy to the stochastic models of dynamic critical phenomena [56], phase field models are often classified into models of type A, B and C. Models of type A describe systems with non-conserved order parameters which evolve according to time-dependent Ginzburg–Landau (or Allen–Cahn) equations [57]. Mod-