Computational Materials Science xxx (2018) xxx–xxx

Contents lists available at ScienceDirect

Computational Materials Science

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

Phase-field analysis of volume-diffusion controlled shape-instabilities in metallic systems-II: Finite 3-dimensional rods

P.G. Kubendran Amos [a,b,*], L.T. Mushongera [a], Tobias Mittnacht [b], Britta Nestler [a,b]

[a] Karlsruhe University of Applied Sciences, Institute of Materials and Processes (IMP), Moltkestr. 30, 76133 Karlsruhe, Germany
[b] Institute of Applied Materials (IAM-CMS), Karlsruhe Institute of Technology (KIT), Strasse am Forum 7, 76131 Karlsruhe, Germany

ARTICLE INFO

Article history:
Received 4 October 2017
Received in revised form 19 December 2017
Accepted 20 December 2017
Available online xxxx

Keywords:
Shape-instabilities
Spheroidization
Rods
Ovulation
Satellite particles
Phase-field modelling

ABSTRACT

Three-dimensional rods form an integral part of the microstructure in materials with high applicability like eutectoid composites. Morphological evolution of the these rods, governed by its inherent difference in the curvature, is analysed by employing a thermodynamically consistent phase-field model in this work. Similar to the study of 2D plate-like structures, an analytical approach is extended to comprehend the kinetics of this volume-diffusion governed transformation. Despite the agreement of the theoretical treatment with the 2D simulations, the onset of contra-diffusion, a behaviour which has been shown to be absent in two-dimension, introduces a progressive deviation from the expected kinetics. However, a simplified relation between the time-taken for the spheroidization $\left(\frac{\tau}{\tau'}\right)$ and the aspect-ratio of the 'capped' rod $\left(\frac{w}{t_p}\right)$ is attained from the outcomes of the phase-field simulation, which is expressed as $\frac{\tau}{\tau'} \approx 5.8\left(\frac{w}{t_p}\right)^2$. The phase-field study is further extended to analytically ill-posed but physically observed 'uncapped' and 'faceted' rods, to understand the mechanism of its transformation and subsequently, analytical expressions are obtained to predict the transformation kinetics of these rods. Moreover, it is uncovered that irrespective of the initial configuration of the rod (faceted or otherwise), capped rods form an intrinsic part of the morphological evolution.

In complete agreement with the experimental observations, present study determines the critical aspect-ratio $\left(\frac{w}{t_p} = 8\right)$, above which the spheroidization involves the breaking-up of the rods ('ovulation'). The formation of 'satellite' particle(s) which introduces coarsening into the morphological evolution of the rods is also analysed. Furthermore, it is identified that the distance between the spheroids (d_s), after ovulation and coarsening, follows a definite relation proportional to the height of the rod (w), given by $d_s \approx 0.0143w^{1.71}$.

1. Introduction

Phase transformations influenced by the interplay of several thermodynamical parameters yield interesting microstructures [1]. These microstructures are meticulously engineered by suitable solidification and/or heat-treatment techniques to render desired properties. Eutectic composites are one such category of materials with a unique microstructure which are frequently sought for its applicability in robust environments [2]. A conventional eutectic composite comprises of a ductile matrix reinforced with precipitate-rods. This microstructure is generally achieved, either, by solidification [3,4] or independently, through fiber-reinforcement [5]. The geometrical feature of the rods, which governs the strengthening of the matrix, is significantly influenced by the manufacturing technique and also by the crystallographic orientation-relation between the constituent phases [6,7].

Despite the potential of these eutectic composites, stability of the rods at high temperature poses an imminent threat to its applicability. Owing to its morphology, under appropriate thermodynamical conditions, these rods undergo transformation which ultimately leads to their dissociation [8]. Although favoured in few instances due to the change in properties that accompany [9–11], these morphological changes are ill-preferred during applications [12,13]. Thus, both theoretical [14–16] and experimental [17–19] attempts are made to understand the mechanisms and kinetics of this transformation. Theoretically, these rods are categorized as finite [20,15] and infinite [21–23] to adopt suitable analytical approach. Depending on the physical system considered, pertinence of this consideration varies. Inspired by the works of Plateau [24] and Rayleigh [25], Nichols and Mullins postulated a numerical treatment [26], through the delineation of the thermo-

* Corresponding author.
E-mail address: prince.amos@kit.edu (P.G. Kubendran Amos).

https://doi.org/10.1016/j.commatsci.2017.12.046
0927-0256/© 2017 Elsevier B.V. All rights reserved.

dynamical principles (Gibbs-Thomson effect) involved, which predicts the stability of the rods under an imposed perturbation [27]. This approach has been enhanced by averting the mathematical delineation and analysing the transformation in accordance with the distribution of the chemical-potential [28,14]. Phase-field studies have employed both these approaches separately to provide a significant understanding on the factors influencing the stability of the rods [29,30]. Regardless of these advancements, few assumptions and un-addressed aspects mitigate the reach of the current understanding to the physical systems [31]. Thus, in this work, an attempt is made to bridge some of these gaps by quantitatively analysing the volume-diffusion governed shape-instabilities in finite-rods using thermodynamically-consistent phase-field model [32,33]. Since the phase-field parameters and the model remain same for both parts of the current analysis, readers are directed to part-I for an understanding of the model and its thermodynamical coherence.

2. Spheroidization of 3-dimensional rods

2.1. Analytical prediction of spheroidization kinetics in 'capped' rods and deviation introduced by 'contra-diffusion'

A cementite (θ) rod with circular cross-section and hemispherically-capped longitudinal ends, as shown in Fig. 1 at an initial time step $\tau = 0$, is introduced into ferrite matrix (α). For all the simulations in the present work, the diameter of the rod t_p is retained at 0.012 μm, while its length w is appropriately varied to achieve the desired aspect-ratio. Any phase transformation amongst these two solid phases α and θ is impeded by assigning equilibrium composition and subsequently, conserving the volume of the evolving phase. Furthermore, the physical values corresponding to the parameters, like diffusivity (D), molar-volume (Ω) and interfacial-energy (γ_s), that govern the transformation are collectively presented in Table 1. The 'capped' rod is allowed to evolve, driven entirely by the inherent difference in the curvature, without the influx of any external perturbations. In accordance with Ref. [35], the driving-force at the beginning of the transformation, Γ_0 is written as

$$\frac{\Gamma_0}{\tau'} = \frac{4\pi n t_p}{(2w + \pi t_p - 4r_c)}, \tag{1}$$

where $\tau' = \frac{D\Omega^2 c^{\theta}_{eq}\gamma_s}{\kappa T}$, w and t_p are the geometrical features of the rod as depicted in Fig. 1. n is a constant that accounts for the number of diffusion paths while κ is the Boltzmann's constant. c^{θ}_{eq} refers to the equilibrium composition of evolving phase (*cementite*) obtained from CALPHAD and temperature, T is considered to be 973 K. r_c is the radius of the resulting sphere which through the constraint of volume-preservation is $r_c = \left(\frac{t_p^2}{16}(2t_p + 3w)\right)^{\frac{1}{3}}$.

As shown in Fig. 1, the rod of aspect-ratio 6, assumes an ellipsoidal shape with a major-axis $2a$ and equal minor-axes $2b$ at the midpoint of the transformation $\left(\tau_{\frac{1}{2}}\right)$. For a 3-dimensional ellipsoid, the principal radii of curvature reads [36,37]

$$R_1 = \frac{1}{H - \sqrt{H^2 - K}} \tag{2}$$

$$R_2 = \frac{1}{H + \sqrt{H^2 - K}} \tag{3}$$

where H is the mean curvature and is expressed as

$$H = \frac{ab^2\left(3a^2 + 5b^2 + (a^2 - b^2)(\cos 2\theta - 2\cos 2\phi \sin^2\theta)\right)}{8\left(a^2b^2\cos^2\theta + b^2\sin^2\theta(b^2\cos^2\phi + a^2\sin^2\phi)\right)^{\frac{3}{2}}} \tag{4}$$

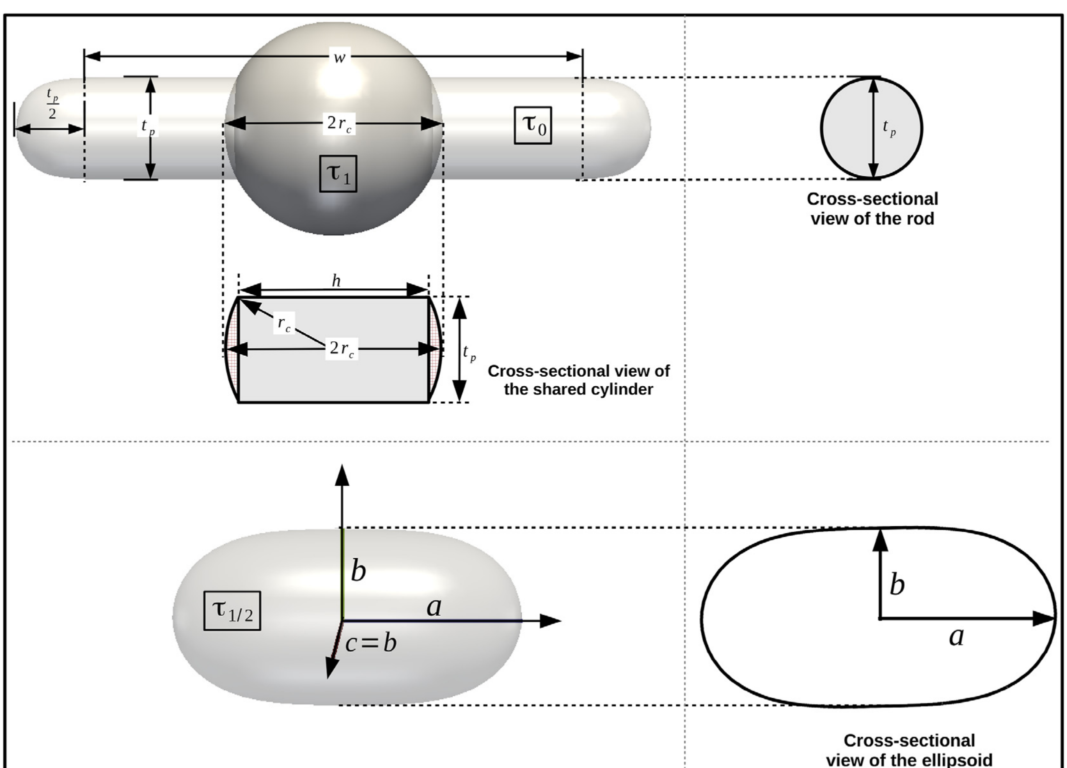

Fig. 1. Morphology of the 3D capped rod at the beginning (τ_0), midpoint $\left(\tau_{\frac{1}{2}}\right)$ and end (τ_1) of the transformation, along with its corresponding cross-section. The cross-section of the shared cylinder is also isolated and depicted. The geometrical notations involved are declared.

Please cite this article in press as: P.G. Kubendran Amos et al., Comput. Mater. Sci. (2018), https://doi.org/10.1016/j.commatsci.2017.12.046