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Phase-field study of the transient phenomena induced by 'abnormally' large grains during 2-dimensional isotropic grain growth

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ABSTRACT

'Abnormally' large grains, whose sizes are greater than twice the critical radius ($2R_c$), are known to alter the isotropic grain growth phenomena. In the present work, phase-field simulations of 2-dimensional microstructures are extensively analysed to elucidate the deviations from the normal grain growth introduced by the presence of abnormal grains. Polycrystalline microstructures that are 'artificially' made to resemble physical structures, by governing the distribution and the sizes of the abnormal grains, is employed to analyse the grain growth in the presence of large grains. This study unravels that the abnormal grains induce a period of transition during which its grain size distribution is shifted and confined within $2R_c$, indicating a complete disappearance of the abnormality in the microstructure. Furthermore, it is identified that this transition period establishes a bimodal distribution, which subsequently evolves into a unimodal time-invariant distribution. This behaviour noticeably reveals the misconception that the disappearance of the abnormality signifies the onset of normal grain growth. Moreover, despite the apparent disappearance of the abnormal grains, a continued increase in the volume-fraction of these 'pre-existing' abnormal grains is recognized, and in the steady-state condition, it is observed that the microstructure predominantly consists of these pre-existing abnormal grains. Influence of the factors like initial volume-fraction of the abnormal grains F_o and degree of abnormality $\overline{U}_{max}$ on the duration of the transient period is quantified by investigating close to hundred microstructures with unique F_o and $\overline{U}_{max}$.

1. Introduction

In the absence of phase transformation, microstructural evolution in polycrystalline material is governed by the thermodynamical ability of the system to reduce its grain boundary energy per unit volume. Owing to the extensive influence of the microstructure on the behaviour of the material, grain growth is analysed both theoretically and experimentally, to gain substantial understanding. Despite the influence of several factors, geometrical and topological, which convolute the dynamics of grain growth, it is identified that the grain size distribution remains unaltered all through the evolution during normal grain growth [1–3]. This time-invariant behaviour is frivolously accounted by the consideration that the entire evolution is governed by the difference in the principle curvature and thus, the larger grains grow at the expense of the smaller ones without noticeably disturbing the size distribution. Hillert, in his seminal work, invokes this consideration and presents an analytical treatment for grain growth as a special case of Ostwald ripening [4]. Accordingly, the approach postulated by Lifschitz and Slyozov [5] and Wagner [6] is extended to encapsulate the evolution of grains in a polycrystalline system. In addition to several other deductions, this approach yields a size distribution function of the form

$$P(u) = \frac{\beta u}{(2-u)^{2+\beta}} \cdot (2e)^{\beta} \cdot \exp\frac{-2\beta}{2-u}, \tag{1}$$

where $u = R/R_c$ with R and R_c representing the radius of the grain and the critical radius above which transition from shrinkage to growth occurs, respectively. In a 2-dimensional set up, the parameter $\beta = 2$ and $R_c = \overline{R}$, while in 3D ($\beta = 3$) this relation is expressed as $R_c = 9/8\overline{R}$. In 2D, 'normal' grain growth, characterized by the distribution function in Eq. (1), posits a restriction that maximum grain size can never be greater than twice the average grain size, owing to its mathematical stability. Thus, it was postulated that 'abnormally' large grains with geometrical feature $R > 2R_c$ grow predominantly at the expense of other smaller grains disrupting the time-invariant distribution [4]. However, subsequent theoreti-

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cal studies on pure polycrystalline systems which overlook the influence of crystallographic orientation and pinning, show that the size-advantage of the 'abnormally' large grains (referred to abnormal grains henceforth) does not induce 'abnormal' grain growth, wherein few grains grow at the expense of the others. On the contrary, it has been identified that the abnormal grains induce a transient period during which the evolution tends towards steady-state growth [7–9]. Conventionally, this steady-state grain growth is recognized by the time-invariant behaviour of the size distribution and adherence of the growth kinetics to the power law, although few deviations in the power-law have been reported [10].

Microstructures resulting from the manufacturing processes rarely exhibit complete adherence to a well-defined grain size distribution. Therefore, heat treatment techniques that induce grain growth in such polycrystalline structures invariably involve a transition period over which self-similar transformation is achieved [11,12]. Owing to its practical implications, theoretical studies attempting to relate the influence of the initial microstructure on these transient phenomena have increasingly been reported [13,9,14]. Simulation studies in addition to the analytical approaches have been vital in explicating the physics undergirding grain growth. Moreover, initial report on the onset of a transition period in the presence of abnormally large grains, contradicting the view of abnormal grain growth, pertains to Monte-Carlo simulations [7]. Often these early attempts were limited owing to the computational restriction. For instance, the aforementioned simulation study analyses a small regime of the microstructure with a single abnormal grain fixed in the center. However, advancements and increased availability of the computational resources enable the simulation of the polycrystalline structures that resemble physical microstructures. Recently, Zöllner et al. by employing one such advanced simulation technique, (Potts types Monte-Carlo) distinguished and analysed the transient phenomena observed in a supposedly random microstructure [15]. Despite the role of the abnormally large grains in governing the evolution of the microstructures, studies have been predominantly focused on abnormal grain growth induced by difference in the grain boundary energy and mobilites [16–19]. Thus, investigations on the influence of the abnormally large grains on the dynamics of grain growth have not been sufficiently reported yet.

Following its outset, phase-field models have been increasingly adopted to simulate phase transformations including solidifications and solid-state transformations [20]. Apart from being thermodynamically consistent, these models ensure the computational and numerical efficiency by circumventing the need for tracking the interface and replacing it with finite-diffuse interface. This diffuse interface separates the bulk phases and is defined by a smoothly varying function. The evolution of respective phase-field variable corresponds to the observed transformation. Furthermore, asymptotic analyses of these diffuse-interface models have shown to recover the outcomes of sharp-interface models, particularly Gibbs-Thomson effect [21] and the force balance equation at triple junction [22]. Therefore, phase-field studies have proven to be of significant importance in gaining insights into complex microstructural transformation like grain growth, which are otherwise laborious to attain. A recent study comparing the evolution of the phase-field simulation with the in-situ observation of grain growth demonstrates an acceptable degree of convergence between the results [23]. Moreover, theoretical analysis comparing the outcomes of phase-field and Potts Monte-Carlo simulations of isotropic grain growth reveals no significant deviation [24]. Phase-field approach has already been employed in the simulation of abnormal grain growth involving pinning, anisotropic grain boundary energy and mobilities [25–28]. Additionally, substantial insights on inherently complex processes like grain boundary segregation and transition have been obtained through phase-field modelling [29–33]. Thus, in the present work, a thermodynamically-consistent phase-field approach is employed to understand the transient phenomena induced by the size-advantage abnormal grains during the isotropic grain evolution.

2. Simulation set-up

2.1. Phase field model

Microstructural transformation in a physical system, irrespective of its nature, is thermodynamically propelled by the minimization of the underlying free-energy. In this work, a phase-field model based on the free-energy functional $\mathcal{F}$ is employed to simulate the microstructural evolutions [34,35]. Accordingly, the dynamics of the resulting evolution is governed by the minimization of this functional $\mathcal{F}$ which comprises of free-energy contribution from within the grain (bulk phases) and grain-boundary (interface). This free-energy functional of *Ginzburg-Landau type* for a polycrystalline system of N grains is expressed as

$$\mathcal{F}(\boldsymbol{\phi}) = \int_{\Omega} \epsilon a(\boldsymbol{\phi}, \nabla\boldsymbol{\phi}) + \frac{1}{\epsilon} w(\boldsymbol{\phi}) + f(\boldsymbol{\phi}) \mathrm{d}\Omega, \tag{2}$$

where Ω is the volume(area) of the simulation domain under consideration and ϵ is a length-scale parameter that governs the width of the diffuse interface. In Eq. (2), $f(\boldsymbol{\phi})$ is the free-energy contributions from each bulk grain. Identity of the N grains involved in the simulation is encompassed in the functional $\mathcal{F}$ through vector-valued continuous phase-field variable $\boldsymbol{\phi}$ of N components $(\phi_1, \phi_2 \ldots, \phi_\alpha, \phi_\beta, \ldots, \phi_N)$, where ϕ_α is the state variable representing the volume-fraction of individual grain α. Gradient energy density $\epsilon a(\boldsymbol{\phi}, \nabla\boldsymbol{\phi})$ in Eq. (2) is expressed as the summation of pair-wise interactions between the grains, α and β, sharing an interface

$$\epsilon a(\boldsymbol{\phi}, \nabla\boldsymbol{\phi}) = \epsilon \sum_{\alpha<\beta} \gamma_{\alpha\beta} [a_{\alpha\beta}(q_{\alpha\beta})]^2 |q_{\alpha\beta}|^2. \tag{3}$$

Here, $\gamma_{\alpha\beta}$ is the interface energy density of the grain boundary separating α and β. The form adopted by the interface energy is defined by the term $a_{\alpha\beta}$ wherein anisotropy is conventionally introduced to simulate the desired crystal-symmetry based morphology [36]. Furthermore, this formulation of the gradient energy density enables the introduction of orientation relation in the interfacial energy, as opposed to continuum-field model wherein the crystallographic orientation is incorporated in the phase-field [37]. Since, the present works overlooks the contributions from the crystallographic orientation and exclusively considers isotropic evolution, interested readers are directed to Refs. [38,39], for a comprehensive understanding on the inclusion of orientation relation in the present model. In Eq. (3), $a_{\alpha\beta}$ is expressed as a function of gradient vector $q_{\alpha\beta}$ which is written as

$$q_{\alpha\beta} = \phi_\alpha \nabla\phi_\beta - \phi_\beta \nabla\phi_\alpha. \tag{4}$$

In the present model, multi-obstacle potential $w(\boldsymbol{\phi})$ is involved, as opposed to well-known double-well potential, which reads

$$w(\boldsymbol{\phi}) = \frac{16}{\pi^2} \sum_{\alpha<\beta} \gamma_{\alpha\beta} \phi_\alpha \phi_\beta + \sum_{\alpha<\beta} \gamma_{\alpha\beta\delta} \phi_\alpha \phi_\beta \phi_\delta. \tag{5}$$

While all the possible interfaces are encompassed in the first term of Eq. (5), the second term $\phi_\alpha \phi_\beta \phi_\delta$ prevents the formation of 'spurious' or third phase, also referred to as 'ghost' phase, in the grain boundary during the evolution. The thermodynamical consistency of adopting the above formulation of the double-well potential has already been extensively analysed in Ref. [40]. The choice of the parameter $\gamma_{\alpha\beta\delta}$ is made in accordance with the work of Nestler