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Phase-field study on the formation of first-neighbour topological clusters during the isotropic grain growth

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ABSTRACT

Grain growth in polycrystalline material is influenced by numerous factors which convolute the understanding of the process. Present work intends to delineate certain aspects of this complexity by quantitatively analysing the topological evolution of the grains and its first-neighbours resulting from multiphase-field simulations. Upon verifying the consistency of this approach with the existing 2- and 3-dimensional analytical predictions, face-switching events of about 75,000 grains in 3D domain is extensively analysed. Despite the expected numerical dominance of the face-loss event, we find the affinity of this event to decrease with increase in face-class. A transition in 'switching affinity' is observed above face-class 14, wherein, the face-gain events are preferred over loss events. The pathway of the topological evolution is comprehensively analysed to identify its influence on the life-span of the grains. This analysis indicates that the topological evolution around the average face-class, 'dead zone', invariably shortens the life-span of the grains and considerable gain in the face-class is seldom observed. The topological behaviour of the first-neighbours during grain growth is quantitatively captured through a well-known statistical tool called heat-maps. And for the first time, the formation of 'topological clusters' which account for the time-invariant behaviour of the grains is elucidated.

1. Introduction

Understanding the microstructural evolution in a polycrystalline material is of primary interest to both engineers and material scientists alike. Although superficially, the evolution of the polycrystalline material is governed by the simple principle of reducing the grain boundary area, several factors have been reported to play an influencing role [1]. One such factor with a considerable influence on the evolution is the topological nature of the grains. Mathematically, topology, in itself, is an extensive topic. However, in the context of the polycrystalline materials, these studies are often restricted to the number of faces observed in a grain [2–6]. This topological feature is referred to as face-class of a grain which is replaced by edge-class in 2-dimensional cases. Irrespective of the dimensions, this topological feature relates directly to the number of surrounding grains. For instance, in 3D, the face-class of a grain is equal to the number of grains constituting its first neighbour. Thus, when compared to size, this feature inherently includes the nature of its surrounding to certain extent [7–9]. Seminal work of Aboav-Weaire considers face-class of an individual grain and relates it to that of its neighbour [10,11]. Furthermore, the growth rate of a grain in relation to its topological feature is captured by von Neumann-Mullins law [12–14]. This relation, originally postulated for 2D, has been extended to three-dimension by MacPherson and Srolovitz [15]. Moreover, while rendering an extension to Neumann-Mullins result, this work recognizes and includes the influence of geometrical features like mean-width on the kinetics of grain growth. Despite numerous reports on the topological behaviour of the grains, a comprehensive understanding on the temporal evolution of face-class of the grains and its neighbours is yet to be attained [16,17]. Understandably, this inadequacy is primarily due to enormous data-sets that emerge from the evolution of large numbers of grains. Quantitative handling of these data-sets which include both geometrical and topological evolution of the grain and its neighbours is rarely pursued, and is replaced by appropriate mathematical treatment. Although substantial understanding has been gained by this approach, the replacing mathematical-treatments are specifically formulated to address the problem at hand [18–21]. On the other hand, studies considering fewer number of grains to circumvent the complexity of handling huge data deviate noticeably from

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the expected analytical predictions [22]. Thus, unique approach is required to analyse the topological evolution quantitatively considering appropriate number of grains. In this study, the topological evolution of the grains along with its neighbours are quantitatively presented using an appropriate statistical tool [23]. Although this well-known tool called heat-maps is hardly used in the analysis of grain evolution, this work intends to provide a framework by highlighting its importance.

Attempts enhancing the understanding of grain growth extend beyond experimental observations to theoretical studies [24–27]. Approaches that are more pronounced in explicating the microstructural evolution in polycrystalline materials include Phase-field models, Monte Carlo Potts models, Vertex models, Cellular Automata and Front tracking methods [20,28–42]. Recently, the phase-field approach has been excessively involved in simulating the microstructural transformation especially in polycrystalline material [43–45]. Tracking grain boundaries which introduces immense complexity in sharp interface models is appropriately averted by employing suitable phase-field parameters (ϕ_α). Furthermore, the interface (grain boundary), which is usually few atoms in width, is collectively described with mesoscopic bulk phases (grains) by involving a diffuse interface. The consistency of this approach which is verified asymptotically, e.g. [46,47]. Pioneering works on understanding grain growth through phase-field analysis dates back to 1997 [48]. Interestingly, despite of being one of the early studies and confined to 2D, a dedicated work is reported on the topological evolution of the grains. Several advancements are reported frequently on the phase-field study of grain growth, such as the introduction of anisotropy to resemble the physical environment [49,50]. However, recent study comparing the in-situ observation of grain growth in titanium-alloy with the outcomes of an isotropic phase-field simulations indicates that, at least from a statistical standpoint, evolution in an isotropic system holds a close resemblance to the ones observed experimentally [37]. Thus, in the present work, phase-field simulations under isotropic grain boundary properties are statistically analysed with a particular focus on topological evolution.

The remainder of this work unfolds with a brief description of the phase-field model and simulation domain. Outcomes of the present simulations are compared with analytical predictions in the following Sections 3.1 and 3.2. Subsequently, the influence of the first neighbour on the geometrical and topological evolution of a grain is elucidated in Section 3.3. Different face switching events that characterize the topological evolution of individual grains are described in Section 3.4.1 with their influence on life-span in Section 3.4.2. In Section 3.5.1 temporal evolution of the first-neighbours are captured through the tool 'heat-maps' and the formation of clusters are presented in Section 3.5.2.

2. Simulation set-up

2.1. Phase-field model

Grain growth in polycrystalline systems is driven by the thermodynamical ability to reduce the grain boundary area per unit volume. The current study employs a phase-field approach wherein the minimization of free energy functional, $\mathcal{F}$ implicitly contributes to this driving force by the attempt of minimizing curvature. Although, complete description of this model is available elsewhere [51], a concise elucidation is given in this section.

The free energy functional, $\mathcal{F}$ of *Ginzburg-Landau type*, over a domain volume Ω in a system of N distinct grains, is generally expressed as

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

where $\boldsymbol{\phi}$ is the vector-valued continuous phase-field variable of N components $(\phi_1, \phi_2 \ldots, \phi_\alpha, \phi_\beta, \ldots, \phi_N)$ and ϕ_α is the state variable representing the volume-fraction of grain α. ϵ is a length-scale parameter that governs the diffuse-interface width and $f(\boldsymbol{\phi})$ is the free-energy contribution from the bulk phase within the grain. However, since the present transformation is entirely governed by the reduction in the interfacial or grain boundary area, this contribution form within the grain is overlooked by considering $f(\boldsymbol{\phi}) = 0$ [44].

The contribution $a(\boldsymbol{\phi}, \nabla\boldsymbol{\phi})$ is the gradient energy density written as the summation of the pair-wise interface contributions from grains, α and β expressed as,

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

$a_{\alpha\beta}$ in the above Eq. (2), expressed as the function of $q_{\alpha\beta}$, defines the form of interfacial energy of evolving grain-boundary, where in anisotropy can be introduced.

The gradient vector, $q_{\alpha\beta}$ involved in this formation, is generalized by

$$q_{\alpha\beta} = \phi_\alpha \nabla\phi_\beta - \phi_\beta \nabla\phi_\alpha \tag{3}$$

and $\gamma_{\alpha\beta}$ denotes the interfacial energy density of the grain boundary between the α and β grains.

The multi-obstacle potential $w(\boldsymbol{\phi})$ involved in Eq. (1) reads

$$w(\boldsymbol{\phi}) = \frac{16}{\pi^2} \sum_{\alpha<\beta} \gamma_{\alpha\beta} \phi_\alpha \phi_\beta + \sum_{\alpha<\beta} \gamma_{\alpha\beta\delta} \phi_\alpha \phi_\beta \phi_\delta, \tag{4}$$

wherein, $w(\boldsymbol{\phi})$ is set to ∞ if $\boldsymbol{\phi}$ is not on the Gibbs simplex

$$\mathcal{G} = \left\{ \boldsymbol{\phi} \in \mathbb{R}^N : \sum_\alpha \phi_\alpha = 1, \phi_\alpha \geqslant 0 \right\}. \tag{5}$$

This condition induces a sharp defined minima for the bulk-phases when compared to the multi-well potential. Furthermore, first of the double-summation in Eq. (4) encompasses all possible α/β combinations while the second, triple summation of higher order terms $\phi_\alpha \phi_\beta \phi_\delta$ prevents the generation of 'spurious' or 'ghost' phase, a third phase, in a two-phase boundary. To understand the numerical and computational efficiency of this obstacle-potential, readers are directed to Refs. [44,46,52].

The corresponding evolution equation adopts the form,

$$\tau\epsilon \frac{\partial\phi_\alpha}{\partial t} = \epsilon\left[\nabla \cdot a_{,\nabla\phi_\alpha}(\boldsymbol{\phi}, \nabla\boldsymbol{\phi}) - a_{,\phi_\alpha}(\boldsymbol{\phi}, \nabla\boldsymbol{\phi})\right] - \frac{1}{\epsilon} w_{,\phi_\alpha}(\boldsymbol{\phi}) - \lambda \tag{6}$$

where derivatives with respect to ϕ_α and $\nabla\phi_\alpha$ of the energy terms are presented as $a_{,\phi_\alpha}, a_{,\nabla\phi_\alpha}$ and $w_{,\phi_\alpha}$. Moreover, the constraint $\sum_{\alpha=1}^{N} \phi_\alpha = 1$ is locally sustained by introducing the Lagrange multiplier, λ

$$\lambda = \frac{1}{N} \sum_{\alpha=1}^{N} \left[\epsilon\left[\nabla \cdot a_{,\nabla\phi_\alpha}(\boldsymbol{\phi}, \nabla\boldsymbol{\phi}) - a_{,\phi_\alpha}(\boldsymbol{\phi}, \nabla\boldsymbol{\phi})\right] - \frac{1}{\epsilon} w_{,\phi_\alpha}(\boldsymbol{\phi}) \right] \tag{7}$$

The parameter τ denotes the mean of the local mobilities $(\tau_{\alpha\beta})$ calculated by

$$\tau = \frac{\sum_{\alpha<\beta} \phi_\alpha \phi_\beta \tau_{\alpha\beta}}{\sum_{\alpha<\beta} \phi_\alpha \phi_\beta} \tag{8}$$

In all the simulations, a constant value is assigned to τ to sustain the kinetically isotropic nature of the microstructural evolution. Additionally, parameters involved in the phase-field evolution equation are appropriately non-dimensionalized to ensure the numerical efficiency and to emphasize the underlying physics.