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An advanced level set approach to grain growth – Accounting for grain boundary anisotropy and finite triple junction mobility

C. Mießen *, M. Liesenjohann, L.A. Barrales-Mora, L.S. Shvindlerman, G. Gottstein

Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, 52056 Aachen, Germany

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ABSTRACT

The novelty of the proposed level-set approach to grain growth resides in the explicit consideration of structural interfacial elements of the microstructure. The extensions allow to consider anisotropic grain boundary energies and triple junction drag in polycrystalline materials. The simulated predictions were compared to analytical expressions for the growth rate of grains under the influence of a finite triple junction mobility with excellent agreement.

1. Introduction

Subsequent to recrystallization, polycrystals undergo grain growth during annealing. Grain growth is driven by the elimination of grain boundary surface to minimize the free energy of the polycrystal. It proceeds by the motion of the grain boundaries (GB) towards their center of curvature and induces a continuous topological rearrangement. This process is decisive for the properties of the resulting microstructure after heat treatment and consequently for the macroscopic properties of crystalline materials.

In an ideal isotropic system, where grain boundary motion is only affected by the local curvature, GB migration leads to a minimization of the total GB in the polycrystal. This evolution is often described as a motion by mean curvature of the GBs [1–7]. In an anisotropic scenario, the evolution of the GB network obeys to different rules of energy dissipation. Dihedral angles at triple junctions depart now from 120° due to different energy densities of adjacent GBs. Additionally, grain boundary motion can also be affected by their possibly distinct mobilities [8–10]. This interplay is reflected in the way microstructure evolution proceeds concomitantly with a change in the misorientation distribution function (MODF) [7]. Furthermore, as shown recently in several investigations [13,11,12,8,14], the properties of triple junctions (TJ) can decisively influence microstructure evolution especially in ultra-fine grained or nanocrystalline materials and lead normally to different grain growth kinetics [15,16].

Due to the restrictions and difficulties to study experimentally dynamic processes in nanocrystalline materials, a considerable number of investigations [13,17–23] have been carried out by means of computer simulations. For this task, several models have been developed. They can be roughly separated into two classes based on their deterministic or probabilistic approach to represent microstructure evolution. Vertex models (VM) [13,17,20,24–27], phase field models (PFM) [28–31] and level-set models (LSM) [4,5,7] are examples of deterministic algorithms, whereas in the class of probabilistic approaches the Monte Carlo Potts models (MCP) [18,19,32] are widely used.

It is also possible to classify deterministic models in the way a microstructure is internally represented. For instance, in vertex or network models only the GBs and their junctions are discretized but not the interior of the grains. In these models, a grain is defined by the volume enclosed by the grain boundaries. In contrast, phase field and level-set methods discretize the volume of the polycrystal and thus, they do only represent microstructural elements such as grain boundaries, triple lines and quadruple junctions implicitly. The abstraction of the microstructure in network models, such as VMs, allows a clear interpretation of the physics of grain growth however at the cost of high computational complexity due to the necessity of implementing rules for topological transformations. On the other hand, in most models where a volume discretization is utilized, the topological transformations are solved automatically by a natural constraint prohibiting overlaps and free space. In these models, however, the topological features are not resolved explicitly and thus effects stemming from structural elements other than the GBs need to be modeled in roundabout ways. We

* Corresponding author.
E-mail address: miessen@imm.rwth-aachen.de (C. Mießen).

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propose an algorithmic solution to fill this apparent gap in existing grain growth models and demonstrate the consideration of finite, in particular low mobilities of TJ in a 2D level-set framework.

A level-set model for grain growth was introduced by Elsey, Esedoglu Smereka in [7]. They factorized the motion by mean curvature by varying the convolution kernel along the GBs. The challenge of utilizing level-set functions to represent the microstructural evolution of a polycrystal is due to the simultaneous tracking of the isosurface and the affecting scalar field, describing the anisotropy of the GBs on each grid point in an area around the interface. In contrast to VMs, the GB is not an explicit object in PFM or LSM models. The representative implicit function always needs to inherit the structural property of the original GB at each grid point. For this reason, VMs were already successfully extended [13,17] to consider the effect of finite TJ mobilities in 2D and quadruple junction mobilities in 3D.

Regarding level-set methods, the model developed by Elsey et al. [5,7] shows great potential due to its computational efficiency and long term stability in 3D. For this reason, in the present contribution, this model was further developed to consider the effect of grain boundary junctions.

The current algorithm was designed for parallel computer architectures by dividing the microstructure into its smallest possible object, i.e. grains. A grain-object stores the corresponding level-set functions, its position in space, and the local topology. Since most of the operations in the level-set approach are applied at a grain level, it is possible to create independent computational tasks and utilize an OpenMP parallelization approach to reduce considerably the time-to-solution. The parallelization is not further discussed in the present contribution but will be published elsewhere [33]. The grain growth level-set (GraGLeS++)[1] simulation tool is provided as open source code.

In the present contribution, we utilized a parallel algorithm to study the effect of finite triple junction mobilities on 2D grain growth. For this, we first analyze the evolution of a four-sided crystal in a well defined environment and compare it to the predictions of an analytical expression derived in [13]. Results on the behavior of different topological classes of an evolving polycrystalline network are discussed subsequently. Finally, the grain growth kinetics of large-scale simulations will be presented and discussed - with special emphasis on the effect of the transient time and initial microstructure on the kinetic growth exponent.

2. Level-set algorithm

Since this method was introduced by Osher and Sethian [1], it has been successfully applied to a vast number of physical processes that involve interface motion. The level-set method is a mathematical framework to describe surfaces and their evolution with time. The method uses an implicit real-valued function ($\phi(t,x)$) that is evaluated on a fixed Cartesian grid. The isosurface with level zero or *zero level-set* of the implicit function describes the position of the surface (Γ):

$$\Gamma := \{x \in \Omega \,|\, \phi(0,x) = 0\} \subset \Omega \tag{1}$$

Note, that the zero level-set is a subset of the domain Ω, where the function ϕ was defined on. Instead of computing the motion of the parameterized surface, the idea of the method is to track the evolution of the implicit funtion with time. The position of the surface can be always identified as the zero level-set at time $t > 0$.

In order to couple the motion of different phases, these algorithms utilize a "Predictor–Corrector" procedure, where the motion of individual objects is first locally performed and then globally corrected. Originally, the model was only able to simulate ideal grain growth. Only recently, it was enhanced by Elsey et al. [5] to consider different grain boundary energies.

In this section, we present a new level-set algorithm for the simulation of anisotropic grain growth in polycrystalline materials, considering the effect of finite triple junction mobilities in two dimensions.

2.1. Level-set framework - the evolution of individual surfaces

To begin with, we want to link the evolution of a single closed surface to the evolution of a unique level-set function. Therefore, let $\Gamma(0) \subset \Omega \subset \mathbb{R}^2$ be an initial closed surface inside the domain Ω and

$$e[\Gamma] = \int_\Gamma \gamma(n_\Gamma(x))\, dx \tag{2}$$

denote the energy of a surface. $\gamma : \Gamma \to \mathbb{R}$ is a phenomenological function of unit normal vectors, describing the energy density per unit area on the surface. The energy minimization inevitably leads to the evolution of such surface. Thus, any point $x \in \Gamma(t)$ on the surface at a certain time t will move in its normal direction $n_\Gamma(t,x(t))$ with a velocity:

$$v(t,x(t)) = m(n_\Gamma(t,x(t)))\,\gamma\,\kappa(x), \tag{3}$$

where m denotes the mobility of a point $x(t) \in \Gamma$ [34].

Given the initial closed surface Γ_0, we define a function $\phi(t,x)$ on $\mathbb{R}^2 \times \{t \geqslant 0\}$, which fulfils Eq. (1). Thus, the isosurface with level 0 of the function $\phi(t,x)$ describes the position of the initial closed surface. Such a function is called the level-set function. Since numerous functions meet this requirement an additional constraint is needed to ensure uniqueness of $\phi(t,x)$:

$$|\nabla\phi| = 1,\ \forall x \in \Omega. \tag{4}$$

Thus, the level-set function gives the distance to the nearest point on its zero level set for each $x \in \Omega$. Such function is called a signed-distance function and it will be referred to as d. In terms of the signed-distance function, we can describe the unit normal by

$$n = \frac{\nabla\phi}{|\nabla\phi|} = \nabla d \tag{5}$$

and the curvature of the isosurface by

$$\kappa = \nabla \cdot n = \nabla \cdot \left(\frac{\nabla\phi}{|\nabla\phi|}\right) = \nabla \cdot (\nabla d). \tag{6}$$

By construction of the total derivative of $\Gamma(t)$ we obtain an equation of motion for the level-set function:

$$\frac{\partial\phi(t,x(t))}{\partial t} - \nabla\phi(t,x(t)) \cdot \frac{\partial x(t)}{\partial t} = 0 \tag{7}$$

$$\iff \frac{\partial\phi(t,x(t))}{\partial t} - \nabla\phi(t,x(t)) \cdot v(x(t))\,n(x(t)) = 0 \tag{8}$$

Utilizing the velocity defined in Eq. (3), we obtain the well-known level-set function:

$$\frac{\partial\phi}{\partial t} - v_n|\nabla\phi| = 0. \tag{9}$$

Eq. (9) allows us to track the evolution of an implicit function instead of the original surface. At first hand, this might be perceived as too laborious but the advantages will become clearer in the following.

[1] https://github.com/GraGLeS/GraGLeS2D.git.