Computational Materials Science 89 (2014) 233–241

Contents lists available at ScienceDirect

Computational Materials Science

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

Development of a level set methodology to simulate grain growth in the presence of real secondary phase particles and stored energy – Application to a nickel-base superalloy

Andrea Agnoli [a,b,*], Nathalie Bozzolo [a], Roland Logé [a,c], Jean-Michel Franchet [b], Johanne Laigo [b], Marc Bernacki [a]

[a] Mines ParisTech, CEMEF – Centre de Mise en Forme des Matériaux, CNRS UMR 7635, CS 10207 rue Claude Daunesse, 06904 Sophia Antipolis cedex, France
[b] Snecma Gennevilliers, 171 boulevard Valmy, 92702 Colombes, France
[c] Thermomechanical Metallurgy Laboratory – PX Group Chair, Ecole Polytechnique Fédérale de Lausanne (EPFL), Rue de la Maladière 71B – CP 526, CH-2002 Neuchâtel, Switzerland

ARTICLE INFO

Article history:
Received 3 December 2013
Received in revised form 18 March 2014
Accepted 25 March 2014
Available online 18 April 2014

Keywords:
Grain growth
Finite element
Zener pinning
Simulation
Microstructure
Level set

ABSTRACT

The influence of secondary phase particles on grain growth (Zener pinning) is simulated in two dimensions using a level set method. Several simulations with circular particles are performed to study the influence of particle surface fraction and distribution. The limiting grain sizes are compared to previous numerical simulations from literature. It is shown that the method allows to take into account the morphology of real particles as measured by microscopy. Moreover, the model also allows to introduce stored energy driven grain boundary migration in Zener pinning simulations.

1. Introduction

In microstructures containing secondary phase particles Zener pinning [1] is the phenomenon that hinders grain growth, eventually leading to a limiting grain size. The understanding and modeling of Zener pinning is of great interest as it is practically exploited to control and limit grain size in several industrial alloys. During the last six decades, the phenomenon has been widely studied and many different analytical models have been proposed in the literature (see [2] for a comprehensive review). Despite the variety of all these studies, there is a global agreement that the limiting grain size can be predicted by this general relation:

$$\overline{R} = K\frac{\overline{r}}{f^m}, \tag{1}$$

where $\overline{R}$ is the average radius of grains, $\overline{r}$ and f are respectively the average radius and the volume fraction of the secondary-phase particles. K and m are two parameters that fluctuate according to the assumptions that are made to obtain the equation.

In the literature the pinning effect of secondary phase particles on grain growth has already been modeled by Monte Carlo, phase-field and boundary-tracking methods. Monte Carlo models [3–5], which were the first to be developed, and phase-field models [6–8], which have gained more attention in the last years, are able to simulate both the 2D and 3D Zener pinning phenomenon. On the contrary, boundary-tracking models are limited to 2D simulations [9] or to 3D simulation of the interaction of a single grain boundary with particles [10,11]. Overall, while all methods can effectively simulate Zener pinning in the simple case of circular or spherical particles, there is not yet a model that can deal with particles whose shape is more complex than ellipsoidal. In addition, all models still assume that particles are incoherent with the matrix, that is the interface energy between grains and particles is isotropic. The present paper introduces the simulation of Zener pinning based on a level set description of interfaces in a finite element context. It is to note that the level set approach has been also developed in the context of uniform grids with a finite difference formulation [12,13]. The numerical approach presented in this work was already used to simulate both 2D and 3D primary recrystallization [14] and grain growth [15] in polycrystals in a finite element context where anisotropic meshing and adaptive remeshing techniques were used. In the conference paper [16], first

* Corresponding author at: Mines ParisTech, CEMEF – Centre de Mise en Forme des Matériaux, CNRS UMR 7635, CS 10207 rue Claude Daunesse, 06904 Sophia Antipolis cedex, France. Tel.: +33 0493957415.
E-mail address: andrea.agnoli@mines-paristech.fr (A. Agnoli).

http://dx.doi.org/10.1016/j.commatsci.2014.03.054
0927-0256/

numerical simulations of pure grain growth with second phase particles in context of level set approach were introduced. However the numerical methodology described was limited to 2D Zener pinning without stored energy, with isotropic boundary energy and without a real validation comparatively to other numerical approaches or to classical limiting grain size analytical models. The main advantage of this technique compared to other numerical methods is the possibility to treat the particle–grain boundary interaction explicitly (through the direct effect on grain boundary curvature). Purpose of the present paper is to extend this level set framework in order to take into account the morphology of the second phase particles, the anisotropy of the interface energy and also to introduce stored energy driven grain boundary migration in Zener simulations. This last aspect seems quite interesting to study those microstructural phenomena where the Zener pinning force is of the same order of magnitude as the stored energy driving force for boundary migration [17].

2. Numerical model

In the level set approach, the function ϕ is defined as the signed distance d from an interface Γ of a sub-domain G belonging to a domain Ω. The distance is evaluated on each interpolation point of the considered finite element mesh. The sign of ϕ is defined positive inside the sub-domain (i.e. a grain) and negative outside. Then, the level 0 of ϕ allows to determine the considered interface (i.e. a grain boundary):

$$\begin{cases} \phi(x) = (\chi_G(x) - \chi_{\overline{G}}(x))d(x,\Gamma), \quad x \in \Omega \\ \Gamma = \{x \in \Omega, \phi(x) = 0\}, \end{cases} \tag{2}$$

where χ_G and $\chi_{\overline{G}}$ are, respectively, the characteristic functions of G and the complement of G. *A priori*, if a microstructure contains N_G grains, then one level set function (ϕ_i) per grain G_i has to be considered.

If capillarity is considered as the only driving force for grain growth, assuming a constant boundary mobility (M) and energy (γ), the kinetic law for the grain boundary Γ_i of the grain G_i can be described as:

$$\vec{v}_i = -M\gamma\kappa_i\vec{n}_i, \tag{3}$$

where $\vec{n}_i = -\frac{\nabla\phi_i}{\|\nabla\phi_i\|}$ and $\kappa_i = \nabla\cdot\vec{n}_i$ correspond, respectively, to the outside unit normal and the mean curvature of Γ_i in the sense of fluid mechanics (i.e. equal to the curvature in 2D and equal to the sum of the two principal curvatures in 3D). It is to note that, as $\vec{n}_i$ (and so κ_i) varies along the boundary Γ_i, then the calculated value of $\vec{v}_i$ for grain i varies as well along the grain boundary. Then, capillarity driven microstructure evolution is described by the following set of convection equations:

$$\begin{cases} \frac{\partial\phi_i}{\partial t} - M\gamma\kappa_i\vec{n}_i\cdot\nabla\phi_i = 0 \\ \phi_i(t=0,x) = \phi_i^0(x), \qquad \forall i \in \{1,\ldots,N_G\}, \end{cases} \tag{4}$$

where ϕ_i^0 is the imposed initial distance function of each grain. If all level set functions satisfy the metric property $\|\nabla\phi_i\| = 1$, then the problem of Eq. (4) can be reformulated as a set of diffusion equations, where the explicit calculation of the curvature and the normal of the grain boundaries can be avoided [15]:

$$\begin{cases} \frac{\partial\phi_i}{\partial t} - M\gamma\triangle\phi_i = 0 \\ \phi_i(t=0,x) = \phi_i^0(x), \quad \forall i \in \{1,\ldots,N_G\}. \end{cases} \tag{5}$$

As the resolution of Eq. (5) can result in values of $\|\nabla\phi_i\|$ different from unity, then it is necessary to reinitialize periodically all level set functions (so that $\|\nabla\phi_i\| = 1$), by solving this set of reinitialization equations:

$$\begin{cases} \frac{\partial\phi_i^*}{\partial\tau} + s_i(\|\nabla\phi_i^*\| - 1) = 0 \\ \phi_i^*(\tau=0,x) = \phi_i(t,x), \qquad \forall i \in \{1,\ldots,N_G\}, \end{cases} \tag{6}$$

where ϕ_i^* is the reinitialized function, τ is a fictional time and s_i is the sign of ϕ_i^*. Eq. (6) is solved in a convective form (with a unitary transport velocity [14]) for a total fictional time τ_{TOT}, which corresponds to the distance (from the zero level of the function) up to which the function is reinitialized. Finally, the simulation of capillarity driven grain growth involves all these steps at each time increment (details for each step are given in [14,15,18]):

1. Grain boundary migration is calculated by solving Eq. (5) for each active level set function.
2. All active level set functions are modified near the grain interfaces to remove vacuum regions appearing at multiple grain junctions [15]: $\phi_i^{**}(t,x) = \frac{1}{2}[(\phi_i(t,x) - \max_{j\neq i}(\phi_j(t,x))]$.
3. All active level set functions are reinitialized (so that $\|\nabla\phi_i\| = 1$ near the grain interfaces), by solving Eq. (6), in a narrow zone around all interfaces which is defined by τ_{TOT}.
4. Negative level set functions all over the resolution domain are defined as non-active in the algorithm, as they correspond to disappeared grains.
5. Anisotropic remeshing is performed when at least one grain boundary leaves the anisotropically meshed layer (that is a narrow zone of anisotropic refined mesh around interfaces).

Stored energy driven grain boundary migration can be introduced in the level set framework by defining a constant energy value e_i for each grain G_i. Then, it is possible to build the velocity field $\vec{v}_E(t,x)$ associated with stored energy differences across grain boundaries as follows [14,18]:

$$\vec{v}_E(t,x) = M\sum_{i=1}^{N_G}\sum_{\substack{j=1\\ j\neq i}}^{N_G}\chi_{G_i}(t,x)exp(-\beta|\phi_j(t,x)|)(e_i - e_j)\vec{n}_j(t,x), \tag{7}$$

where β is a positive parameter calibrated to obtain a negligible exponential term outside the anisotropic mesh surrounding interfaces. The advantage of the velocity field defined by Eq. (7) is that it can be used for all grains and it does not require information concerning the microstructure topology (neighboring grains). Moreover, this formulation allows avoiding kinematic incompatibilities at the multiple junctions [18]. Finally, the problem defined by Eq. (5) can be modified by adding a convection term that takes into account also stored energy driven grain growth:

$$\begin{cases} \frac{\partial\phi_i}{\partial t} - M\gamma\triangle\phi_i + \vec{v}_E(t,x)\cdot\nabla\phi_i = 0 \\ \phi_i(t=0,x) = \phi_i^0(x), \qquad \forall i \in \{1,\ldots,N_G\}. \end{cases} \tag{8}$$

The simulation of capillarity and stored energy driven grain growth involves the same steps that were previously defined for capillarity driven grain growth, except the first one that is replaced by the following two steps:

1a. The velocity field associated with stored energy differences across grain boundaries is calculated using Eq. (7).
1b. Grain boundary migration is calculated by solving Eq. (8) for each active level set function.

It is to note that in order to reduce computation time, the level set functions of non-neighboring grains in the initial microstructure (separated by a certain number of grains) are grouped to form global level set functions (families of grains) that are used to perform the calculation steps described previously for the microstructure evolution. The grouping algorithm, based on graph coloration,