Simulating recrystallization in titanium using the phase field method

S P Gentry and K Thornton
Materials Science and Engineering Department, University of Michigan, Ann Arbor, Michigan, 48109, USA
E-mail: kthorn@umich.edu

Abstract. Integrated computational materials engineering (ICME) links physics-based models to predict performance of materials based on their processing history. The recrystallization phase field model is developed and parameterized for commercially pure titanium. Stored energy and nucleation of dislocation-free grains are added into a phase field grain-growth model. A two-dimensional simulation of recrystallization in titanium at 800°C was performed; the recrystallized volume fraction was measured from the simulated microstructures. Fitting the recrystallized volume fraction to the Avrami equation gives the time exponent $n$ as 1.8 and the annealing time to reach 50% recrystallization ($t_{0.5}$) as 71 s. As expected, the microstructure evolves faster when driven by stored energy than when driven by grain boundary energy.

1. Introduction
Integrated computational materials engineering (ICME) is crucial in advancing material design and optimization. Linking models together will enable simulated parametric studies across length scales, incorporating microstructure into larger-scale component analysis. For example, simulations of static recrystallization are needed for the processing history of metals to be used in microstructural mechanical behavior simulations. As such, successful ICME requires accurate physics-based simulations that predict realistic microstructures.

When metals undergo plastic deformation, a network of dislocations is formed within the microstructure. Increasing the applied stress provides an additional driving force for dislocation motion and creates more dislocations. The increased dislocation density results in a stored energy ($f_{\text{stored}}$) within the microstructure, which is approximated as [1]

$$f_{\text{stored}} = \frac{1}{2} G b^2 \rho$$

(1)

where $G$ is the shear modulus, $b$ is the Burgers vector, and $\rho$ is the dislocation density. Upon heat treatment, metals may undergo recrystallization, in which dislocation-free grains nucleate and grow in the microstructure. Reduction of the stored energy provides the driving force for growth of the new grains. The recrystallization process is both time- and temperature-dependent. Recrystallization is commonly described by an Avrami relation between the fraction recrystallized ($X$) and the annealing time ($t$) [1]. Specifically,

$$X = 1 - \exp \left( -\beta \left( \frac{t}{t_{0.5}} \right)^n \right)$$

(2)
where \( \beta = -\ln(0.5) \), \( t_{0.5} \) is the time to reach a fraction of 50% recrystallized grains, and \( n \) is the time exponent.

In this study, we focus on the microstructural evolution of titanium. Titanium is a lightweight metal that has high strength; predicting its recrystallization kinetics will facilitate alloy development. We seek to demonstrate that a recrystallization phase field model may be employed to predict the microstructural evolution of titanium during thermomechanical processing.

2. Phase Field Model

The phase field method was utilized to model recrystallization and grain growth in a deformed microstructure. The phase field grain-growth model employs a functional to describe the free energy of the system in terms of nonconserved order parameters [2]. Each grain is assigned an identifying number \( i \) and a corresponding order parameter \( \eta_i \). A system with \( N \) grains has \( N \) independent order parameters \( \eta_1, \eta_2, ..., \eta_N \) that are tracked at every point and evolved according to Allen-Cahn dynamics. The total free energy of the system, \( F \), is the volume integral of the free energy density. The recrystallization model includes three contributions to the free energy density with the total free energy given by:

\[
F = \int_V \{ f_{\text{bulk}} + f_{\text{gradient}} + f_{\text{stored}} \} \, dV
\]

where \( f_{\text{bulk}} \) is the bulk free energy density, \( f_{\text{gradient}} \) is the gradient energy density, and \( f_{\text{stored}} \) is the stored energy density. The bulk term is expressed as [3]

\[
f_{\text{bulk}} = m_0 \left[ \sum_{i=1}^{N} \left( -\frac{1}{2} \eta_i^2 + \frac{1}{4} \eta_i^4 \right) + \alpha \sum_{i=1}^{N} \sum_{j \neq i} \eta_i^2 \eta_j^2 + \frac{1}{4} \right]
\]

where \( \alpha = 1.5 \) and \( m_0 \) is a constant related to the grain boundary energy and the diffuse interface width. The gradient energy density penalizes large gradients in the order parameter and is given by

\[
f_{\text{gradient}} = \frac{\kappa}{2} \sum_{i=1}^{N} |\nabla \eta_i|^2
\]

where \( \kappa \) is the gradient energy penalty. The stored energy provides an additional driving force for microstructural evolution. Each grain \( i \) has a corresponding dislocation density \( \rho_i \); the effective dislocation density interpolates the dislocation densities based on the values of the order parameters at that point. We interpolate the effective dislocation density as

\[
\rho_{\text{eff}} (\eta_1, \eta_2, ..., \eta_N) = \frac{\sum_{i=1}^{N} \eta_i^2 \rho_i}{\sum_{j=1}^{N} \eta_j^2}
\]

This is similar to the work of Moelans, Godfrey, Zhang, and Juul Jensen [4, 5], but is generalized to an arbitrary number of grains. The stored energy, Eq. 1, is calculated with the effective dislocation density at a given point, \( \rho_{\text{eff}} \) above, resulting in

\[
f_{\text{stored}} = \frac{1}{2} Gb^2 \rho_{\text{eff}} (\eta_1, \eta_2, ..., \eta_N).
\]

The evolution of the microstructure is given by Allen-Cahn dynamics [6]:

\[
\frac{\partial \eta_i}{\partial t} = -L_i \left( \frac{\delta F}{\delta \eta_i} \right) = -L_i \left( m_0 \left( -\eta_i + \eta_i^3 + 2\alpha \eta_i \sum_{j \neq i}^N \eta_j^2 \right) - \kappa (\theta) \nabla^2 \eta_i - Gb^2 \eta_i \left( \rho_i - \rho_{\text{eff}} \right) \right),
\]

(8)
The partial differential equations are discretized with the finite difference method and evolved using forward Euler time stepping.

Active parameter tracking [7, 8] is employed to reduce the computational expense of the phase field grain-growth model. Each order parameter is only stored where it is above $1 \times 10^{-6}$; otherwise the order parameter is assumed to be zero. The simulation in this work used an algorithm based on the data structure in McKenna and Voorhees’s Anisotropic Phase Field Evolver [9, 10], with this work adding MPI parallelization, stored energy contributions, and recrystallization.

To simulate static recrystallization, new grains are added to the phase field model at the beginning of the simulation. A new order parameter is created for each recrystallized grain and assigned a dislocation density of zero. The order parameter is seeded with a circle at a randomly selected position on a grain boundary or on a triple point. The number of newly seeded grains is based on a predetermined number density of nuclei. For the first $N_{\text{hold}}$ time steps, the order parameters of the new grains are held while the other order parameters adjust. When the hold period is complete, microstructural evolution is allowed to continue as normal.

3. Simulation Parameters

The model has been parameterized for commercially pure titanium that was uniaxially compressed by 20% at room temperature and then annealed at 800°C. The initial recrystallized nuclei density was estimated to be $5.5 \times 10^{12} \text{ m}^{-3}$ from experiments [11]. The grain boundary energy of titanium was taken as 0.7 J/m² for high-angle grain boundaries [12]. The grain boundary mobility at 800°C was extracted from recrystallization experiments and found to be $1.9 \times 10^{-13} \text{ m}^4/\text{Js}$ [11]. The shear modulus was taken to be 25 GPa at 800°C as approximated using the Voigt-Reuss-Hill model [13] from elastic constant measurements of single crystal titanium [14]. The Burgers vector was set to 0.295 nm for an $\vec{a}$ dislocation [15].

The dislocation density in the material can be approximated from [16]

$$\sigma = \sigma_y + M_T C_{\text{stored}} G h \sqrt{\rho}$$

(9)

where $\sigma$ is the applied stress, $\sigma_y$ is the yield stress, $M_T$ is the Taylor factor, and $C_{\text{stored}}$ is a constant that was approximated to be 0.15 from Ref. [17]. For titanium, $M_T$ was taken to be 2.5 according to Ref. [18]. Compression of titanium reduced one dimension of the sample by 20%, corresponding to an applied stress of 582 MPa [11]. The yield stress from experiments was 325 MPa [11]. Using Eq. 9, the average dislocation density was calculated to be $8.6 \times 10^{15} \text{ m}^{-2}$.

For the simulation, the initial microstructural domain was set to a random grain structure with an average grain size of 53 μm arranged on a 1500 × 1500 uniform grid with $\Delta x = \Delta y = 0.5 \mu m$. The time step, $\Delta t$, was set to $3.8 \times 10^{-3} \text{ s}$. Each grain in the initial microstructure was randomly assigned a dislocation density within ±25% of the average dislocation density. The radius of each nucleus was $15\Delta x$ and the hold time ($N_{\text{hold}}$) was 200 time steps, which is sufficient for existing order parameters to adjust for the seeded order parameter. The nuclei number density was converted from three dimensions to two dimensions by assuming that the initial phase fractions of round recrystallized grains would be equal. The number density of nuclei in two dimensions was taken to be $5.5 \times 10^7 \text{ m}^{-2}$.

4. Results and Discussion

The evolved microstructure is shown in Fig. 1 at four annealing times. For visualization, the dislocation density is scaled by the average dislocation density of the initially deformed microstructure ($\rho/\rho_{\text{ave, t=0}}$). Recrystallized grains are white (corresponding to a dislocation density of zero) while the existing grain structure is colored based on the scaled dislocation density. The recrystallized nuclei (16 μm-diameter circles) are visible in the deformed matrix in the first
snapshot taken at 1.9 s (Fig. 1(a)). 70 s of annealing (Fig. 1(b)) results in significant growth in the recrystallized grains, while much less evolution is seen where there are no recrystallized grains. The microstructure is fully recrystallized after 220 s of annealing (Fig. 1(c)). The fraction recrystallized is plotted as a function of time, as shown in Fig. 2. The simulated data was fit to the Avrami equation (Eq. 2) using only the data points between $X_{0.1}$ and $X_{0.9}$. The best fit was obtained for $n$ of 1.8 and $t_{0.5}$ of 71 s for the simulated two-dimensional microstructure.

During annealing there are two competing driving forces for microstructural evolution: stored energy and grain boundary energy. Stored energy differences between adjacent grains cause recrystallized grains to grow at the expense of the deformed grains. The grain boundary energy drives the large grains to grow at the expense of small grains, which reduces the total grain boundary length. During recrystallization, the simulated evolution is dominated by the stored energy contribution as evidenced by the growth of both the small recrystallized grains and larger grains with low stored energy (Figs. 1(a), 1(b), 1(c)). If the microstructural evolution of recrystallization was dominated by the grain boundary energy, then small dislocation-free grains would disappear to reduce the grain boundary length. When recrystallization is complete, only the grain boundary energy drives microstructural evolution because the stored energy is zero. Annealing a fully recrystallized microstructure is then governed by the reduction of the grain boundary energy. From 220 s (Fig. 1(c)) to 3600 s (Fig. 1(d)), the grains grow and the grain

**Figure 1.** Simulated microstructural evolution after annealing at 800°C for 1(a) 1.9 s, 1(b) 70 s, 1(c) 220 s, and 1(d) 3600 s. The colors indicate the scaled dislocation density ($\rho/\rho_{ave,t=0}$); recrystallized grains are white.
boundaries become straighter. The simulation of the microstructural evolution from 0 s to 3600 s shows the effects of both stored energy and grain boundary energy.

The competing driving forces result in different rates for microstructural evolution. The stored energy causes the recrystallized grains to grow quickly, with full recrystallization occurring in 220 s. However, grain growth that occurs after recrystallization is much slower. From 220 s (Fig. 1(c)) to 3600 s (Fig. 1(d)), there were only small changes in the grain sizes. These differences in growth rate occur as a result of the combined model; no changes are made to the evolution equation.

5. Conclusions

This paper presented a model and simulation results for recrystallization and grain growth in metals. The model is based on the phase field method, which takes into account the thermodynamics and kinetics of materials. A polycrystalline microstructure is modeled with a separate order parameter for each grain; these order parameters are evolved according to Allen-Cahn dynamics. The recrystallization phase field model incorporates stored energy contributions and the nucleation of new undeformed grains. The model also retains the driving force due to the reduction of the total grain boundary energy, which leads to grain growth.

The recrystallization phase field model was used to simulate microstructural evolution in two dimensions for deformed titanium. The model was parameterized for commercially pure titanium that was compressed to 20% uniaxial strain and then annealed at 800°C. The recrystallized grains grew at the expense of the deformed grains as expected, and the recrystallized fraction was calculated as a function of time. In the two-dimensional simulation presented, the time exponent of 1.8 and the time to reach 50% recrystallization of 71 s provided the best fit to the Avrami equation (Eq. 2). Recrystallization occurred on a much faster time scale than growth of the dislocation-free grains because the driving force from stored energy is larger than the driving force from grain boundary energy. Recrystallization took 220 s, and annealing for an additional 3400 s only had a small effect on the microstructure.

This work involved simulations in two dimensions only; three-dimensional simulations are ongoing and will allow for direct comparison of experimental and computational microstructures. Simulated three-dimensional microstructures can also be used as inputs to other models such as those that predict microstructure-dependent mechanical behavior, and thus are essential for successful integration of the model into an ICME framework. These models can then be directly integrated so that processing conditions are linked to the stress analysis of a designed part.
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