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Sensitivity analysis of a phase field model for static recrystallization of deformed microstructures

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Abstract

Static recrystallization is a process whereby dislocation-free grains are nucleated in a deformed microstructure, and then newly recrystallized grains grow and consume the previously existing grains. This paper describes a phase field model for static recrystallization, along with details of the implementation and simulation results. Recrystallized grains are seeded utilizing a probability-based method, including a hold time to allow the order parameters to adjust to seeded grains. The nominal simulation time is corrected to account for the nuclei hold and for the time required for a nucleus to grow from its critical size to the seeded size. Microstructural evolution was simulated for two- and three-dimensional systems, and the fraction recrystallized was quantified via Avrami kinetics. The resulting Avrami time exponents were in agreement with the expected values for site-saturated nucleation. The variability in the Avrami parameters was quantified by simulating the recrystallization of the same underlying polycrystalline microstructure but using different seed locations. Additional simulations were performed to determine the influence of the deformed microstructure on recrystallization, specifically investigating the effects of the spatial distribution of the initial dislocation density within the microstructure as well as the morphologies of the polycrystalline microstructure. For the significantly deformed polycrystalline microstructures examined in this work, it is shown that microstructural evolution is primarily driven by stored energy in dislocations rather than grain boundary energy.

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Keywords: Phase field model; Static recrystallization; Microstructure evolution; Avrami kinetics

1. Introduction

The processing of metallic alloys often includes mechanical deformation and thermal treatment. Static recrystallization occurs when a plastically deformed metal is annealed without additional mechanical processing, forming new polycrystalline structures that are nearly free of dislocations. Static recrystallization is an important material phenomenon that affects the microstructure of materials, which in turn has a significant influence on the mechanical properties of materials such as steel, aluminum alloys, copper alloys, and titanium alloys [1]. For example, different thermal treatments during static recrystallization of commercially pure titanium resulted in average grain diameters and Vickers hardnesses (HVs) from 6 μm to 20 μm and 170 HV to 260 HV, respectively [2].

During mechanical processing, polycrystalline metals undergo plastic deformation which results in the formation of a network of dislocations. The stress fields from the dislocations give rise to a stored energy that can be approximated by [3]

$$f_s = \frac{1}{2} \rho G b^2 \quad (1)$$

where f_s is the stored energy density, ρ is the dislocation density, G is the shear modulus, and b is the magnitude of the Burgers vector. Therefore, the regions with high dislocation density are at higher energy states than those with low dislocation density.

When the deformed microstructure is annealed, the system can undergo recrystallization and grain growth. The deformation process causes the formation of a dense network of dislocations with regions of pristine (dislocation-free) grains; these small pristine grains serve as nuclei for the recrystallization. The difference between the stored energies of the deformed grains and pristine grains provides the driving force for recrystallization, wherein new crystals (recrystallized grains) with negligible dislocation density grow at the expense of larger deformed grains. The new polycrystalline structures that emerge have negligible stored energy after they fully recrystallize. Further annealing causes grain growth to occur, which is driven by the reduction in the total grain boundary energy in the system. This causes the average grain size to increase as larger grains grow at the expense of smaller grains, reducing the overall grain boundary energy of the system.

The kinetics of a recrystallization process can be described by the Johnson-Mehl-Avrami-Kolmogorov (JMAK) model, which predicts the transformation kinetics under the assumptions of randomly distributed nuclei in space and constant normal velocities of interfaces both in space and time [4, 5]. The Avrami equation is utilized to relate the fraction transformed, X , and the annealing time (t):

$$X = 1 - \exp\left(-\beta\left(\frac{t}{t_{0.5}}\right)^n\right) \quad (2)$$

where $\beta = -\ln(0.5)$, $t_{0.5}$ is the time to reach $X = 0.5$ (i.e., 50% of the volume transformed), and n is the time exponent. Static recrystallization is commonly approximated by a site-saturated condition [3], in which nuclei are assumed to be randomly distributed and are present at $t = 0$, because the pristine crystalline seeds are already present at the start of the annealing process. In this case, the time exponent is expected to be $n = 1, 2$, or 3 for growth dimensions of one, two, and three dimensions, respectively.

In this paper, we utilize the phase field method to simulate static recrystallization. The phase field method is derived upon kinetics and thermodynamics of materials and can be used to simulate microstructural evolution such as the growth of dendrites [6] and anisotropic precipitates [7]. The recrystallization process involves evolution of complex microstructures resulting from the interplay between multiple driving forces such as stored energy and grain boundary curvature. These driving forces can be incorporated into the phase field model by including terms representing them in the free energy. Thus, the phase field model is well suited to study recrystallization and grain growth.

Researchers have already reported phase field models of recrystallization and their capabilities, but most were restricted to one-dimensional (1D) and two-dimensional (2D) studies. For example, 1D simulations have shown that variations in stored energy density can lead to increased roughness of the boundary of the growing recrystallized grain [8]. They found that the amplitude of stored energy density differences has a larger impact on the grain boundary velocity as compared to the grain boundary energy. Prior work has also demonstrated that phase field models of recrystallization can be linked to other simulation techniques. For instance, works by Takaki et al. and Sreekala et al. have linked recrystallization simulations to crystal plasticity models [9-11] and coarse-grained dislocation density models [12], respectively, but these are limited to small numbers of deformed grains in two dimensions. While these works describe

recrystallization phase field models and have provided useful insight into the behavior of recrystallization, they do not provide the quantitative predictions of three-dimensional (3D) microstructural evolution due to their simulation dimensionality. In contrast, a study by Zhu et al. demonstrated that the phase field model can accurately predict Avrami kinetics in three dimensions [13]. However, additional research is needed to quantify the sensitivity of the model to materials parameters.

Efficiently and accurately simulating recrystallization in three dimensions in polycrystalline materials is challenging. Multigrain phase field simulations can be computationally intensive, but this can be reduced using a data structure that only tracks values that are significant, an approach known as the active order parameter tracking [14, 15]. This technique has been used to simulate grain growth in polycrystalline materials, for example, to compare simulations and experiments in a β -stabilized titanium alloy [16]. Recrystallization modeling has the added challenge in implementing the introduction of new grains into the microstructure. Specifically, the size of the pristine grains can be several orders of magnitude smaller than the deformed grains, making it computationally expensive to simulate recrystallization from initial growth to full recrystallization. For instance, recrystallized grain sizes can be on the order of one to hundreds of microns (e.g., Refs. [17, 18]). The phase-field simulations by Zhu et al. were benchmarked with a low carbon steel with a final grain size of 5 μm [13], but we will show later that Avrami kinetics may not be reproduced for a larger grain size. Despite the challenges of 3D recrystallization simulations, it is important that a 3D phase-field model for simulating recrystallization efficiently and accurately predicts Avrami kinetics for a range of parameters under the ideal condition where the analytical model is valid.

In this paper, we present a phase field model that efficiently simulates static recrystallization and grain growth in three dimensions. Recrystallized grains are seeded utilizing a probability-based algorithm, briefly holding the recrystallized nuclei to allow for the order parameters of the surrounding deformed grains to adjust to seeded grains. The nominal simulation time is corrected to account for the nuclei hold and for the time required for a nucleus to grow from its critical size to the seeded size. The time correction was previously suggested in a cellular automaton model [19], but we further correct it by 2-4% by relating it to the critical nucleus size based on thermodynamics of stored and grain boundary energies rather than assuming the critical size to be zero. The critical nucleus can be 50-200 times smaller than a seeded nucleus, so the

growth time necessary to reach the seed size must be accounted for in order to accurately simulate recrystallization. In three dimensions, this growth time can be on the same order of magnitude as $t_{0.5}$. The growth time can be reduced by using smaller seeded nuclei, but this significantly increases the computational requirements of the simulations. We simulate microstructural evolution for 2D and 3D systems, comparing the resulting Avrami time exponents with the expected values for site-saturated nucleation. We also investigate the impacts of stored energy and grain boundary energy on recrystallization kinetics.

2. Model

2.1. Phase field model with stored energy

A phase field model for static recrystallization and grain growth is built upon several phase field models existing in the literature, including those of Chen et al. [20, 21] and Moelans et al. [22]. The phase field approach describes microstructures using a set of order parameters. For a polycrystalline microstructure with N grains, the i -th grain is represented by η_i , where $i = 1, 2, \dots, N$. The thermodynamics of the system is incorporated using a total free energy functional, $\mathcal{F}$, that consists of the bulk and gradient energy densities, f_{bulk} and $f_{gradient}$, respectively. The field of stored energy density due to deformation is incorporated into the free energy as an additional term, f_s . Thus, the free energy functional is given by

$$\mathcal{F} = \int_V \{f_{bulk} + f_{gradient} + f_s\} dV \quad (3)$$

where V is the volume of the system. Each of the energy density terms will be further detailed below. The microstructural evolution is tracked by following the evolution of the order parameters according to the evolution equation based on the free energy functional.

The bulk energy density in Eq. 3 provides a driving force for grains to fill the simulation domain, while penalizing the nonzero values of multiple order parameters at the same location. The expression for f_{bulk} is as follows [22]:

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

where $\alpha = 1.5$, which is selected such that the order parameter values are symmetrical across an interface. The bulk energy constant m_0 is the energy density coefficient. All grains are energetically equivalent with respect to f_{bulk} . The second term, $f_{gradient}$, prevents the formation of sharp changes in the order parameters and controls the width of the interface (grain boundary, in this case). It is formulated as

$$f_{gradient} = \frac{\kappa}{2} \sum_{i=1}^N |\nabla \eta_i|^2 \quad (5)$$

where κ is the gradient energy penalty coefficient. The parameters, m_0 and κ , depend on the diffuse interface width, a model parameter, and grain boundary energy, a material parameter. The terms f_{bulk} and $f_{gradient}$ incorporate the effects of grain boundary energy and grain boundary curvature on microstructural evolution.

The last energy density term is the stored energy density field, f_s , which provides a driving force for microstructural evolution due to the relatively high dislocation density in deformed grains. While the inhomogeneity of the deformation leads to dislocation density variation both within and across the grains, for simplicity, we assume that the dislocation density is uniform within each grain. Thus, we assign each grain i a uniform dislocation density ρ_i . The dislocation density field, ρ , at each point is obtained from the values of the order parameters and their corresponding dislocation densities using an interpolation function of Moelans, Godfrey, Zhang, and Juul Jensen [8, 23]:

$$\rho(\eta_1, \eta_2, \eta_3, \dots, \eta_N) = \frac{\sum_{i=1}^N \eta_i^2 \rho_i}{\sum_{j=1}^N \eta_j^2}. \quad (6)$$

The stored energy density field varies spatially and is related to ρ by Eq. 1. Prior work by Takaki et al. similarly added a stored energy term to the free energy functional [24], but it was developed for an alternative phase field formulation. Both deformed and pristine grains evolve under the effect of this stored energy, allowing for experimentally observed recrystallization and strain-induced boundary migration [25].

Microstructural evolution is driven by reduction in the total free energy, $\mathcal{F}$, with time. It is simulated by evolving each of the nonconserved order parameters based on Allen-Cahn dynamics [26]:

$$\frac{\partial \eta_i}{\partial t} = -L \left[\frac{\delta \mathcal{F}}{\delta \eta_i} \right], \quad (7)$$

which is also known as the time-dependent Ginzburg-Landau equation [27]. Using the free energy functional (Eqs. 3-6), this equation becomes

$$\frac{\partial \eta_i}{\partial t} = -L \left[m_o \left(-\eta_i + \eta_i^3 + 2\alpha \eta_i \sum_{j \neq i}^N \eta_j^2 \right) - \kappa \nabla^2 \eta_i + G b^2 \frac{\eta_i}{\sum_{j=1}^N \eta_j^2} (\rho_i - \rho) \right] \quad (8)$$

where L is the mobility parameter, which is proportional to the grain boundary mobility.

Simulation parameters are set from material parameters. For polycrystalline grain growth with uniform grain boundary energy (i.e., with no stored energy), Moelans et al. derived the following relationships from the sharp-interface limit [22]:

$$\kappa = \frac{3}{4} \gamma_{gb} l_{gb} \quad (9a)$$

$$L = \frac{4\mu_{gb}}{3l_{gb}} \quad (9b)$$

$$m_o = \frac{6\gamma_{gb}}{l_{gb}} \quad (9c)$$

where γ_{gb} is the grain boundary energy, μ_{gb} is the grain boundary mobility, and l_{gb} is the grain boundary width, a model parameter. We apply these relationships to microstructures with varying stored energy, neglecting the effect of stored energy on the grain boundary width. The grain boundary width is set to $l_{gb} = 4\Delta x$ to provide sufficient numerical resolution over the diffuse interface. The phase field equations are nondimensionalized by dividing energy and distance by m_o and l_o , respectively, where l_o is a length scale of choice. In this work, we choose $l_o = \Delta x = l_{gb}/4$ such that the dimensionless grid spacing is 1. Time is scaled by $1/(m_o L)$, which is the dynamic time scale associated with the length scale l_o . Nondimensionalization yields the following:

$$\kappa^* = \frac{\kappa}{m_o l_o^2} = 2 \quad (10a)$$

$$L^* = \frac{L}{L} = 1 \quad (10b)$$

$$m_0^* = \frac{m_0}{m_0} = 1 \quad (10c)$$

$$x^* = \frac{x}{l_0} \quad (10d)$$

$$t^* = tLm_0 = t \left(\frac{\mu_{gb}\gamma_{gb}}{2l_0^2} \right) \quad (10e)$$

$$f_s^* = \frac{f_s}{m_0} = f_s \left(\frac{2l_0}{3\gamma_{gb}} \right) = \left(\frac{1}{2} Gb^2 \rho \right) \left(\frac{2l_0}{3\gamma_{gb}} \right) \quad (10f)$$

$$\bar{f}_s^* = \left(\frac{\bar{f}_s}{m_0} \right) = \bar{f}_s \left(\frac{2l_0}{3\gamma_{gb}} \right) = \left(\frac{1}{2} Gb^2 \bar{\rho} \right) \left(\frac{2l_0}{3\gamma_{gb}} \right) \quad (10g)$$

where an asterisk (*) indicates a nondimensional variable corresponding to the similarly named dimensional variable. The average dislocation density and stored energy, $\bar{\rho}$ and $\bar{f}_s$, respectively, are simulation parameters that are set based on the underlying deformed microstructure. The dislocation density field can also be nondimensionalized by its average value as

$$\rho^* = \frac{\rho}{\bar{\rho}} \quad (11)$$

where ρ^* is the normalized dislocation density field. The field ρ^* is equal to zero and one in locations with zero and average dislocation density, respectively, and can be larger or smaller than one in deformed grains. Using ρ^* , the spatial dependence of f_s^* can be defined in terms of the average parameters $\bar{\rho}$ and $\bar{f}_s$ as

$$f_s^* = \left(\frac{1}{2} Gb^2 \bar{\rho} \right) (\rho^*) \left(\frac{2l_0}{3\gamma_{gb}} \right) = (\bar{f}_s^*) (\rho^*). \quad (12)$$

The phase field equations are solved using the finite difference method on a uniform 3D grid. A central difference scheme is used for the spatial second derivatives, and the order parameters are evolved with the forward Euler time stepping scheme. A separate order parameter is used for each grain, and each of the new recrystallized grains is assigned a new order parameter.

Active parameter tracking [14, 15], wherein only order parameters $\eta_i(x, y, z) > 1 \times 10^{-6}$ are stored at any grid point, is utilized to ensure computational efficiency. Order parameter values below this cutoff are assumed to be zero. The data structure of the order parameters and the numerical implementation of active parameter tracking are based on work by McKenna and Voorhees [28, 29]. Parallelization is implemented with uniform domain decomposition using Message Passing Interface (MPI).

2.2. Initialization of the recrystallization microstructure

The initial microstructure for a recrystallization simulation is generated through the steps that are detailed in this section. The initialization process requires a 2D or 3D polycrystalline microstructure with each grain represented by a unique order parameter and having a known dislocation density. The recrystallized nuclei are assumed to be present in the initial microstructure since static recrystallization occurs during heat treatment after deformation. This initial microstructure is generated by inserting nuclei into the computational domain prior to beginning time evolution. The following steps are used to initialize the recrystallization microstructure; each step is described further in the subsections.

1. Calculate correction time for nuclei growth
2. Determine the number of nuclei to be seeded utilizing experimental results
3. Select seed positions using a probability-based algorithm
4. Seed nuclei at positions selected in step three
5. Evolve microstructure based on Eq. 8, while holding nuclei for microstructure accommodation
6. Release the hold and continue microstructural evolution.

The equations in this section are provided for dimensional variables, but can be nondimensionalized using Eqs. 10-12.

2.2.1. Correction time for nuclei growth

There is often a disparity between the recrystallization nucleus size and the scale of microstructures to be simulated. Specifically, the critical radius of the recrystallized nuclei can be two to three orders of magnitude smaller than the grain size at the end of the recrystallization process. It is thus impractical to simulate the growth of recrystallized nuclei of this size unless the

physical domain size of the simulation is extremely small. For simulations corresponding to typical experimental images, it is computationally necessary to introduce larger seeds in the microstructure. The seed size, r_{seed} , is selected to be smaller than the grains but sufficiently large to be resolved by the phase field model. The consequence of this larger seed is addressed with the correction explained below.

Physically, the radius of the recrystallized nuclei can be predicted from the Bailey-Hirsch criterion, which accounts for the incremental change in the free energy with respect to size of a nucleus that forms [30]. The change in free energy (not energy densities) is calculated by adding two terms: $-\bar{f}_s dV_{nuc}$ and $\gamma_{gb} dA_{nuc}$, where dV_{nuc} and dA_{nuc} are the change in volume and surface area of the nucleus, respectively. The Bailey-Hirsch criterion defines the critical radius size, r_{BH} , as the radius corresponding to the maximum change in free energy upon formation. This size depends on the number of dimensions in the recrystallization study and is given as:

$$r_{BH} = \frac{(n_{dim} - 1)\gamma_{gb}}{\bar{f}_s} = \frac{2(n_{dim} - 1)\gamma_{gb}}{\bar{\rho}Gb^2} \quad (13)$$

where n_{dim} is the number of dimensions. The final form is obtained using Eq. 1.

To estimate the time required for a recrystallized grain to grow from its critical size to its seeded size, we simulate the growth of a single recrystallized grain embedded in a deformed grain. The recrystallized nucleus is circular (in 2D) or spherical (in 3D) with a radius of r_{seed} , has stored energy density $f_s = 0$, and is centered in the domain representing a deformed grain with constant stored energy density equal to $\bar{f}_s$. Two order parameters are defined: one for the recrystallized grain (denoted by η_{rx}) and another for the deformed grain that surrounds it. The radius of the recrystallized grain is measured from the center of the recrystallized grain, where $\eta_{rx} = 1$, to the location along the x-axis where $\eta_{rx} = 0.5$, linearly interpolating between grid points. The initial recrystallized grain size is chosen to be large enough to yield a constant growth velocity, V_{gb} , and thus V_{gb} is determined by performing a linear regression of the recrystallized grain size as a function of time. The seed growth time, t_{seed} , is then given by

$$t_{seed} = \frac{r_{seed} - r_{BH}}{V_{gb}}. \quad (14)$$

This growth time is utilized to correct the simulation time for many-grain simulations, providing the scientific rationale for the time delay postulated by Marx et al. in their cellular automata model

[19]. The seed growth time is a simple estimate and assumes that all nuclei have the same size, rather than the distribution of sizes expected in a deformed microstructure. The growth time also neglects the Gibbs-Thomson effect, assuming the growth velocity is constant even when the recrystallized grain size is close to r_{BH} . Furthermore, t_{seed} is calculated assuming a homogeneous deformed grain surrounding the nuclei; effects of the polycrystalline microstructure are neglected. However, as demonstrated in Section 4, this approximation provides sufficient correction to reproduce Avrami kinetics even though nuclei are preferentially located on grain boundaries or triple junctions and t_{seed}^* is within an order of magnitude of $t_{0.5}^*$. If $t_{0.5}$ is to be compared to experiments, then the seed size should be set such that t_{seed} is substantially smaller than $t_{0.5}$.

2.2.2. Number of nuclei

The number density of nuclei, n_{REX} , may be estimated from experimental grain size measurements [17]:

$$n_{REX} = \left[\frac{4}{3} \pi \left(\frac{D_{REX}}{2} \right)^3 \right]^{-1}, \quad (15)$$

where D_{REX} is the average grain size when recrystallization is complete. This expression assumes that the number of grains in the recrystallized microstructure is equal to the number of initial recrystallized nuclei. The number density and domain size are used to calculate the number of recrystallized nuclei to be placed in the deformed microstructure in the next step.

2.2.3. Position of seeds

Recrystallized nuclei are seeded in the microstructure using a nucleation algorithm, which can be designed such that the nucleation probability is enhanced in the interior of the grains, grain boundaries, or triple junctions. Experimental observations have demonstrated that nucleation is more likely on grain boundaries than within the interior of grains away from grain boundaries under uniform deformation [3]. Additionally, new recrystallized grains have been observed at both two- and three-grain boundaries [31]. It has been postulated that nucleation of second phases may be preferred at triple junctions over two-grain boundaries; these locations in the initial microstructure are more energetically favorable for nucleation than two-grain boundaries due to the larger grain boundary area per volume near the three intersecting grain boundaries [32]. Thus,

we assume that recrystallized nuclei similarly prefer triple junctions over two-grain boundaries. Accordingly, we select seed positions so that nuclei are placed on grain boundaries, slightly favoring triple junctions over two-grain boundaries. However, the approach described below can easily be modified to implement other forms of nucleation probability, for example, where regions with high strain gradient serve as nucleation sites. Prior work on a level set model developed an adaptable, probability-based algorithm for selecting seed positions [33], but here we select the positions using the order parameters of a phase field model.

A stochastic scheme is used for seeding nuclei. The grain boundaries and triple junctions are identified by summing the gradients of all order parameters at position $\mathbf{r}$, $\sum_{i=1}^N |\nabla \eta_i(\mathbf{r})|$. This term is normalized by its smallest and largest values within the simulation domain, $\min(\sum_{i=1} |\nabla \eta_i(\mathbf{r})|)$ and $\max(\sum_{i=1} |\nabla \eta_i(\mathbf{r})|)$, respectively. The maximum value occurs near triple junctions because the sum of three order-parameter gradients is larger than the sum of two gradients, even though each individual gradient has slightly smaller gradients. The relative probability of nucleation with respect to that at a triple junction is implemented by

$$P(\mathbf{r}) = \frac{\sum_{i=1} |\nabla \eta_i(\mathbf{r})| - \min(\sum_{i=1} |\nabla \eta_i(\mathbf{r})|)}{\max(\sum_{i=1} |\nabla \eta_i(\mathbf{r})|) - \min(\sum_{i=1} |\nabla \eta_i(\mathbf{r})|)}, \quad (16)$$

which provides the likelihood of a new grain forming at that position as compared to triple junctions. P is approximately 1.0 on or near a triple junction, approximately 0.86 on grain boundaries away from triple junctions, and is zero within a grain.

The positions of the seeded nuclei centers are selected sequentially. A random point is selected on the domain ($\mathbf{r}_{rand}$) and a random number, Y_{rand} , is generated between zero and one inclusive. If $Y_{rand} \leq P(\mathbf{r}_{rand})$, then a nucleus is seeded at $\mathbf{r}_{rand}$. This process is repeated until the desired number of nuclei based on the experimentally determined density has been achieved.

2.2.4. Nuclei insertion in domain

Each of the nuclei positions selected in step 3 is seeded by inserting a round nucleus into the simulation domain, centered at the nucleus position. The initial value of a nucleus order parameter is given by the following function:

$$\eta_i = \frac{1}{2} \left(1 - \tanh \left(\frac{d - r_{seed}}{2\Delta x} \right) \right) \quad (17)$$

where d is the distance from position $\mathbf{r}$ to the center of the seeded nucleus and Δx is the grid spacing.

2.2.5. Nuclei hold

After seeds are inserted into the phase field domain, the simulation of microstructural evolution commences. An initial hold period is utilized to allow the surrounding microstructure to adapt to the new grains. Order parameters of deformed grains evolve according to Eq. 8, while order parameters of recrystallized grains are kept constant. This approach is similar to that of Jokisaari et al. [34] for seeding second-phase particles, preventing unphysical behavior arising from overlapping order parameters. The hold time, t_{hold} , should be negligible in comparison to the total evolution time.

2.2.6. Continuation of multigrain simulation

When the hold period is complete, the simulation is continued as described by Eq. 8. The nominal simulation time, t_{nom} , is equal to zero at the beginning of the hold, but recrystallization does not commence until after the hold is complete. The corrected simulation time, t_{corr} , is calculated employing the correction terms from Sections 2.2.1 and 2.2.5:

$$t_{corr} = t_{nom} + t_{seed} - t_{hold}. \quad (18)$$

3. Phase field parameters

This paper presents simulations of recrystallization based on nondimensionalized equations with the parameters selected based on recrystallization in commercially pure titanium. The model system was cold-worked titanium that had a dislocation density of $\bar{\rho} = 4.83 \times 10^{15} \text{ m}^{-2}$; recrystallization occurred when the material was annealed at 800°C. The shear modulus was approximated to be $G = 25 \text{ GPa}$, using the Voigt-Reuss-Hill model [35] to estimate the isotropic polycrystalline parameter from the single-crystal titanium stiffnesses measured at 800°C [36]. The grain boundary energy was set to $\gamma_{gb} = 0.7 \text{ J/m}^2$, a value for high-angle grain boundaries in titanium [37] calculated using the disclination-structural-unit model of grain boundaries, and the magnitude of the Burgers' vector for a $\langle 11\bar{2}0 \rangle$ dislocation was taken to be $b = 0.295 \text{ nm}$ [38]. Based on experimental results [39], the grain boundary mobility was taken to be

$\mu_{gb} = 1.9 \times 10^{-13} \text{ m}^4/\text{Js}$ and the recrystallized grain diameter was estimated from micrographs to be $D_{REX} = 7.0 \times 10^{-5} \text{ m}$. The simulation employed $l_0 = \Delta x = 0.5 \times 10^{-6} \text{ m}$, resulting in the following nondimensional parameters: $\Delta x^* = 1$, $\kappa^* = 2$, $L^* = 1$, $m_0^* = 1$, and $\bar{f}_s^* = 2.5$. For numerical stability, the simulation time step, Δt^* , for recrystallization was set to 1×10^{-3} and 2.5×10^{-4} in two and three dimensions, respectively. The hold time, t_{hold}^* , was set to $200\Delta t^*$, corresponding to times of 0.75 s and 0.19 s for two and three dimensions, respectively. The 2D simulations in Section 5.1 were continued after recrystallization was complete and grain growth became the sole mechanism of microstructural evolution. At this transition, Δt^* was increased to 1×10^{-2} ; this time step yielded numerical stability for grain growth simulation and no artifacts were observed from the change. The number density of nuclei in three dimensions was calculated from D_{REX} using Eq. 15 to be $n_{REX} = 5.5 \times 10^{-12} \text{ m}^{-3}$, which corresponds to $n_{REX}^* = 6.9 \times 10^{-7}$. In two dimensions, the initial volume fraction of recrystallized grains was set equal to that in three dimensions, yielding number densities of $n_{REX} = 5.5 \times 10^{-7} \text{ m}^{-2}$ or $n_{REX}^* = 1.4 \times 10^{-5}$. The seeded recrystallized grains had $r_{seed} = 15\Delta x = 7.5 \text{ }\mu\text{m}$. Periodic boundary conditions were employed for all simulations.

The single-recrystallized-grain simulations (Section 2.2.1) employed initial conditions of a circular or spherical recrystallized grain embedded in a deformed grain. A circular or spherical grain with radius $15\Delta x$ ($= 7.5 \text{ }\mu\text{m}$) was created with a sharp interface, and then a brief relaxation period was applied to obtain order parameters with a smooth interface. The normalized dislocation densities of the deformed grain and nucleus were one and zero, respectively. Both 2D and 3D simulations were performed to supply the values of t_{seed}^* for the corresponding multigrain simulations.

The initial condition for a microstructure-scale simulation was a set of equiaxed grains. Nuclei were randomly seeded into an empty domain (without any order parameters), then evolved without stored energy until grains formed [28]. The initial microstructure for 2D simulations had 174 grains with an average grain size of $105\Delta x$ ($= 50.2 \text{ }\mu\text{m}$) on a 1500×1500 grid, which corresponds to a simulation domain of $750 \text{ }\mu\text{m} \times 750 \text{ }\mu\text{m}$. The initial 3D microstructure contained 439 grains with an average grain size of $50.2\Delta x$ ($= 25.1 \text{ }\mu\text{m}$) on a $400 \times 400 \times 400$ uniform grid, or a $200 \text{ }\mu\text{m} \times 200 \text{ }\mu\text{m} \times 200 \text{ }\mu\text{m}$ simulation domain.

Most of the microstructure-level simulations utilized a $\pm 25\%$ variation in the dislocation density, and therefore ρ_i was randomly assigned between $0.75\bar{\rho}$ and $1.25\bar{\rho}$ inclusive; the results

are presented in Sections 4.1 and 4.2. Two exceptions are discussed in Section 5.1, in which we examine a case with a uniform dislocation density and stored energy density ($\rho_i = \bar{\rho}$ and $f_s = \bar{f}_s$) for all deformed grains, and another case with a single deformed grain with a uniform stored energy density.

The fraction recrystallized was calculated periodically during the simulation, counting the fraction of grid points where the largest order parameter was that of a recrystallized grain. The fraction recrystallized was plotted versus time. Avrami parameters were determined by fitting only phase fractions between 0.10 and 0.90 to an alternate form of Eq. 2:

$$\ln(-\ln(1 - X)) = \ln K + n \ln t. \quad (19)$$

For a transformation given by Eq. 2, plotting the left side of Eq. 19 versus $\ln t$ yields a line where the slope is equal to the Avrami exponent, n , and the y-intercept is $\ln K$. The constant K is related to $t_{0.5}$ by

$$t_{0.5} = \left[\frac{-\ln(0.5)}{K} \right]^{1/n}. \quad (20)$$

This equation can be applied to either dimensional or nondimensional times.

4. Results: Multigrain simulations

4.1. Recrystallization in two dimensions

Recrystallization was simulated for a 2D multigrain microstructure utilizing the parameters given in Section 3. We previously demonstrated that the simulated static recrystallization kinetics in two dimensions can be fit to Avrami kinetics [40]. However, the results in this paper demonstrate the correction time is important for accurately characterizing the recrystallization dynamics.

The correction time for the 2D simulations was calculated following the method described in Section 2.2.1. As described earlier, the growth of a recrystallized grain was simulated, and its radius as a function of time was obtained from the distance between the center of the grain and the interpolated location along the x-axis at which $\eta_{rx} = 0.5$. The radius of the recrystallized grain increased linearly over time, as shown in Figure 1. The simulated data are shown in black circles, and the line is the linear least-squares fit to the data. The linear relationship ($R^2 = 0.99998$) indicates the nondimensional grain boundary velocity was constant (at 5.08), suggesting that the JMAK analysis can be applied because its assumption that grain boundary velocity is constant is

met. Utilizing Eq. 13, the critical radius size, r_{BH}^* , was determined to be 0.266. In comparison, the seeded nucleus had $r_{seed}^* = 15$. The seed growth time, t_{seed}^* , was found to be 2.9 using Eq. 14. The hold time, t_{hold}^* , was 0.200 and thus the total correction time, $(t_{seed}^* - t_{hold}^*)$, was 2.7.

Figure 1. Radius of a circular recrystallized grain embedded in a deformed grain as a function of time. The circles are the simulated data, and the line is the linear least-squares fit of the radius versus time. The data is nondimensional and the fit has an R^2 value of 0.99998.

The positions of the recrystallized nuclei were selected with the stochastic algorithm described in Section 2.2.3. Figure 2 shows the relative probability of forming a nucleus at different positions in a subset of the initial microstructure. As set by Eq. 16, $P(\mathbf{r})$ was zero inside of the grains, had a value of one on the triple junctions, and was equal to 0.86 on grain boundaries.

Figure 2. Relative probability, P , of forming a nucleus at different locations in the microstructure. For clarity, only 1.8% of the computational domain is shown.

The nuclei were seeded at the selected points and then the microstructure was evolved to full recrystallization. The microstructural evolution is depicted in Figure 3, where the structures are shown at three points in time: $t_{corr}^* =$ (a) 3.7, (b) 22.7, and (c) 63.7. The time has been corrected for nucleus growth and hold; the microstructure began to evolve without restrictions at $t_{corr}^* = 2.7$. The colors indicate the dislocation density; the gray regions representing grain boundaries were determined from the sum of the squares of the order parameters. At $t_{corr}^* = 3.7$ (Figure 3(a)), thirty-one recrystallized grains (white regions) are present in the microstructure, matching the number density of recrystallized grains calculated from parameters in Section 3. All recrystallized grains were located on grain boundaries or triple junctions, as specified in the model. After evolving the microstructure without restrictions from $t_{corr}^* = 2.7$ to $t_{corr}^* = 3.7$, the diameter of the recrystallized grains increased approximately 25% as compared to the initial nuclei. By $t_{corr}^* = 3.7$, the order parameters have settled to their steady-state profiles after accommodating the new grains. Over time, the recrystallized grains grew and began to impinge on each other, as shown in Figure 3(b) at $t_{corr}^* = 22.7$; the fraction recrystallized was 0.51 at that time. At $t_{corr}^* = 63.7$ (Figure 3(c)), the microstructure was fully recrystallized. Additionally, all grain boundaries evolve from the influence of stored energy, interfacial energy, and grain boundary curvature, as given by Eq. 8 and discussed in Ref. [40]. These images are similar to those presented in our previous paper [40], but the microstructure in Figure 3 utilizes new nuclei locations and incorporates time corrections.

Figure 3. Simulated recrystallized microstructures at three values of t_{corr}^* : (a) 3.7, (b) 22.7, and (c) 63.7. Recrystallization is complete at a time of 63.7. The color bar on the right indicates the normalized dislocation density in all three images; deformed grains are colored and recrystallized grains are white. Grain boundaries are represented by gray shading.

The fraction recrystallized was measured from the multigrain simulation and is plotted against both the uncorrected and corrected time in Figure 4. The Avrami parameters were

determined by fitting the results in Figure 4 to Eq. 19. Without corrections, the Avrami time exponent, n , and $t_{0.5}^*$ were 1.80 and 19.4, respectively. Incorporating time corrections, $t_{seed}^* - t_{hold}^* = 2.7$, the corrected n was 2.10 and $t_{0.5}^*$ was 22.4, which are both larger than the uncorrected values. The goodness of fit, R^2 , also increased from 0.9982 to 0.9999 when time corrections were included, indicating that the fit was improved by the corrections.

Figure 4. Area fraction recrystallized as a function of nondimensional time, utilizing the 2D microstructure in Figure 3. The crosses and the circles correspond to the data obtained from the simulation shown in Figure 3 with and without time corrections, respectively. The least-squares fit of Eq. 19 to the data are given by the solid and dashed lines, corresponding to one simulation with and without time corrections, respectively.

To quantify the variability of the Avrami parameters, the simulation was repeated five additional times. The same deformed microstructure was employed, but nuclei were seeded each time using different random numbers. The time exponent, n , was found to be 2.00 ± 0.11 and $t_{0.5}^*$ was 23.4 ± 1.2 , where the stated errors are the standard deviations for the time exponent and $t_{0.5}^*$, denoted σ_n and $\sigma_{t_{0.5}^*}$, respectively. For comparison, a simulation of a single, pristine grain in a random, coarse-grained dislocation density had $n = 2.05 \pm 0.03$ [12], where the error was determined from the fit of a single run to Eq. 2. Our variability was calculated from six simulations with many nuclei in a polycrystalline microstructure, so a larger variability was expected. The phase field model described in Section 2 yielded reproducible recrystallization kinetics when the number of nuclei and underlying microstructure remained constant. Furthermore, the time exponent of 2.00 ± 0.11 was in agreement with the expected time exponent for site-saturated nucleation and growth, which has an expected value of two in two dimensions [3]. The agreement

between the time exponents indicates that the recrystallization phase field model yields results that are consistent with static recrystallization theory.

4.2. Recrystallization in three dimensions

Recrystallization was also simulated in three dimensions utilizing the simulation parameters provided in Section 3. The single-recrystallized-grain simulation described in Section 2.2.1 was repeated in three dimensions to determine the time correction for this case. The behavior was identical to the results in two dimensions: the radius increased linearly over time with a nondimensional grain boundary velocity of 5.09. The similar results are expected because the grain boundary velocity is dominated by stored energy rather than energy due to curvature. The 3D critical radius, r_{BH}^* , was 0.533, which was twice as large as the value in 2D due to the dimensional dependence of Eq. 13. Utilizing $r_{seed}^* = 15$ and $\Delta t^* = 2.5 \times 10^{-4}$, t_{seed}^* and t_{hold}^* were 2.8 and 0.050, respectively. The total correction time, $(t_{seed}^* - t_{hold}^*)$, was 2.85.

Three-dimensional microstructural evolution is shown in Figure 5 and the corresponding simulated Avrami curve is given in Figure 6. The simulated microstructures are presented for three levels of recrystallization: $X = 0.03$, 0.53, and 1.00, corresponding to $t_{corr}^* = 3.8$ (Figure 5(a)), 10.8 (Figure 5(b)), and 22.8 (Figure 5(c)), respectively. As in Figure 3, the colors indicate the dislocation density and the grain boundaries are shown in gray. The undeformed grains grew at the expense of the deformed grains, as expected. Fitting the simulated data presented in Figure 5 to Eq. 19 yielded an Avrami time exponent of 3.12 and $t_{0.5}^*$ of 10.5. Without corrections, n was 2.13 and $t_{0.5}^*$ was 7.51; thus, time corrections significantly change the Avrami parameters. The exponent obtained with the corrected time, $n=3.12$, is in agreement with the expected value of $n=3$ for site-saturated nucleation in three dimensions within the uncertainty, assuming that the uncertainty in the 3D simulation is similar to that of the 2D simulation (standard deviation of 0.11 for n). The agreement between the expected and simulated values of n in both two and three dimensions supports the validity of the phase field model in Section 2 for use in simulating static recrystallization. This validated model offers future opportunities to examine more complex cases such as recrystallization with clustered nuclei or larger grain sizes.

Furthermore, time corrections are necessary for accurately simulating Avrami kinetics in a range of materials systems. In some systems, these may be negligible, such as the results from Zhu et al. for a low carbon steel. Their 3D simulations predicted an Avrami time exponent of 2.98

without using time corrections [13]. However, we postulate the corrections were not necessary since their final grain size was less than an order of magnitude larger than the critical radius, as calculated using their simulation conditions. In contrast, our 3D simulation had an average recrystallized grain radius that was 65 times larger than the critical radius, 35 μm and 0.533 μm , respectively; the uncorrected $t_{0.5}^*$ was only 2.6 times larger than the seed growth time. For efficient simulations, time corrections should be included for systems where the recrystallized grain size is significantly larger than the critical radius.

Figure 5. Simulated 3D microstructures after times of $t_{corr}^* =$ (a) 3.8, (b) 10.8, and (c) 22.8.

Figure 6. Volume fraction recrystallized as a function of nondimensional time for a simulation shown in Figure 5. The circles indicate the simulated data incorporating $t_{seed}^* - t_{hold}^* = 2.8$, with the dashed line indicating the least-squares fit to the data using Eq. 19. The uncorrected simulation data is indicated with crosses and the fit is given by the solid line.

4.3. Computational requirements

Length-scale bridging decreases the computational resources required for the simulations. The seeded nuclei with $r_{seed}^* = 15$ in the 2D simulation were significantly larger than the nondimensionalized Bailey-Hirsch radius of 0.266. Seeding nuclei of the Bailey-Hirsch radius would have required a mesh that was 56 times finer than the one used, resulting in a computational time requirement that would be approximately 3100 times larger. It was not feasible to decrease the simulation domain size, as this would have further reduced the number of recrystallized nuclei in the simulation. The most computationally intensive simulation in this paper was the 3D simulation described in Section 4.2, which required high-performance computing resources. On the Stampede cluster of the Extreme Science and Engineering Discovery Environment (XSEDE) [41], the simulation took a wall time of 18.0 hours on 256 processors, requiring 4602 core-hours to complete.

5. Results: Parametric study

5.1. Effect of underlying microstructure

Three simulations were compared to determine the sensitivity of the model to variations in the underlying polycrystalline microstructure. The reference simulation (Case 1) was a 2D multigrain simulation randomly selected from the six repeated simulations in Section 4.1. This simulation had 174 deformed grains assigned a dislocation density between $(1 \pm 0.25)\bar{\rho}$. The second simulation (Case 2) used the same microstructure and seeded nuclei but instead assigned the same dislocation density to all deformed grains. The third microstructure (Case 3) contained one large deformed grain with uniform dislocation density within which recrystallized grains were seeded. All three cases used identical positions for seeding the 31 nuclei.

The differences in the initial microstructure were found to give rise to variations in the recrystallization kinetics. A plot of the area fractions recrystallized over time is shown in Figure 8, and the Avrami parameters are given in Table 1. Compared to the reference simulation (Case 1, with dislocation density randomly assigned to 174 deformed grains), all of the time exponents were within one standard deviation ($\sigma_n = 0.11$); the values of $t_{0.5}^*$ were within 1.5 times the standard deviation ($\sigma_{t_{0.5}^*} = 1.22$). Variations in the Avrami parameters between the three cases can be attributed to changes in the dislocation density and the underlying polycrystalline microstructure, consistent with results from Sreekala et al. that varied the network of dislocations

and found n ranged from 1.50 and 2.09 [12]. Recrystallization proceeds slightly slower for the simulation with random dislocation density (Case 1) as compared to the simulation with uniform dislocation density. This is similar to the simulation results from Zhu et al. [13] who stated that the longer recrystallization times are caused by slower grain boundary velocities in regions with lower stored energy. Additionally, Case 2 recrystallizes faster than Case 3 since the grain boundaries in Case 2 provide a small but non-negligible driving force for the growth of recrystallized grains in addition to the stored energy. This indicates that the presence and shape of grain boundaries influence the recrystallization kinetics, even though behavior is dominated by average stored energy.

Figure 7. Simulated area fraction recrystallized versus t_{corr}^* for three variants of the underlying polycrystalline microstructure. The solid curve shows the fraction recrystallized for a random microstructure (with 174 deformed grains having randomly assigned dislocation density). The dotted curve is for the case with the same deformed grain structure but with a uniform dislocation density in the underlying microstructure. The dashed curve is for a single deformed grain with uniform dislocation density. All simulations are seeded with nuclei of recrystallized grains in identical locations.

Table 1. Avrami parameters for the recrystallization curves shown in Figure 7.

	$t_{0.5}^*$	n
Case 1: Randomly assigned ρ^* with 174 grains	21.7	2.15
Case 2: Uniform ρ^* with 174 grains	20.7	2.26
Case 3: Uniform ρ^* with a single grain	23.3	2.14

5.2 Effect of grain boundary energy and stored energy

The sensitivity of the model to grain boundary energy and average stored energy was also investigated. Here, the same normalized dislocation density field, ρ^* , is used for all cases, but $\bar{f}_s^* = \bar{f}_s(2l_0/3\gamma_{gb})$ is set according to the value of $\bar{f}_s$ using Eq. 10(g). The baseline simulation (Case 1) was taken to be the 174-grain microstructure with randomly assigned dislocation density, presented in Section 5.1. The simulation had a grain boundary energy of $\gamma_0 = 0.7 \text{ J/m}^2$ and initial average stored energy of $\bar{f}_s = \bar{f}_{s,0} = 5.3 \times 10^6 \text{ J/m}^3$. The grain boundary energy was $0.5\gamma_0 = 0.35 \text{ J/m}^2$ and $2\gamma_0 = 1.4 \text{ J/m}^2$ for Cases 4 and 5, respectively, with average stored energies of $\bar{f}_{s,0}$. Cases 6 and 7 set $\bar{f}_s$ to $0.5\bar{f}_{s,0} = 2.6 \times 10^6 \text{ J/m}^3$ and $2\bar{f}_{s,0} = 10.5 \times 10^6 \text{ J/m}^3$, respectively, while holding the grain boundary energy constant at γ_0 . These parameters are summarized in Table 2 along with the values of t/t^* and $\bar{f}_s^*$ as calculated using Eqs. 10(e) and (g).

Table 2. Material parameters γ_{gb} and $\bar{f}_s$, nondimensional $\bar{f}_s^*$, time scaling ratio t/t^* , and Avrami parameters $t_{0.5}^*$ and n for cases with different grain boundary energy and average stored energy.

	$\gamma_{gb} \text{ (J/m}^2\text{)}$	$\bar{f}_s \text{ (J/m}^3\text{)}$	$\bar{f}_s^*$	$t/t^* \text{ (s)}$	$t_{0.5}^*$	n
Case 1	$\gamma_0 = 0.7$	$\bar{f}_{s,0} = 5.3 \times 10^6$	2.5	3.76	21.7	2.15
Case 4	$0.5\gamma_0 = 0.35$	$\bar{f}_{s,0} = 5.3 \times 10^6$	5.0	7.52	26.7	2.06
Case 5	$2\gamma_0 = 1.4$	$\bar{f}_{s,0} = 5.3 \times 10^6$	1.25	1.88	18.2	2.22
Case 6	$\gamma_0 = 0.7$	$0.5\bar{f}_{s,0} = 2.6 \times 10^6$	1.25	3.76	36.5	2.22
Case 7	$\gamma_0 = 0.7$	$2\bar{f}_{s,0} = 10.5 \times 10^6$	5.0	3.76	13.0	2.06

The four new cases only required two additional sets of simulations. When the simulation parameters are nondimensionalized (Eqs. 10(e) and (g)), t^* and $\bar{f}_s^*$ are proportional to $\mu_{gb}\gamma_{gb}$ and

$\bar{f}_s/\gamma_{gb}$, respectively; the remaining nondimensional parameters are independent of the material. Thus, this work only needed one set of simulations (one single-recrystallized-grain simulation and one polycrystalline simulation) for two cases with identical $\bar{f}_s/\gamma_{gb}$, provided that time was rescaled. In this section, all reported results are nondimensionalized on the same time scale as Case 1 so that simulation results can be directly compared throughout the paper; this time scale maintains the notation t_{corr}^* . The results for Cases 4 and 7 were obtained from a single simulation with $f_s^* = 5.0\rho^*$. Case 7 had the same time scale as Case 1, while Case 4 was post-processed by rescaling the time. The ratio t/t^* was twice as large for Case 4 as compared to Cases 1 and 7, and therefore Case 4 was rescaled as $t_{corr}^* = 2t_{corr,0.5\gamma_0}^*$, where $t_{corr,0.5\gamma_0}^*$ is the original corrected time scaled with $\gamma_{gb} = 0.5\gamma_0$. Similarly, Cases 5 and 6 used a different simulation with $f_s^* = 1.25\rho^*$, rescaling the time for Case 5 as $t_{corr}^* = 0.5t_{corr,2\gamma_0}^*$ where $t_{corr,2\gamma_0}^*$ is the corrected time scaled with $\gamma_{gb} = 2\gamma_0$. Rescaling nondimensional simulations was computationally efficient as only two sets of simulations were required for the four cases.

The Avrami parameters are given in Table 2 and were calculated by fitting the scaled data to Eq. 19. As expected, rescaling a nondimensionalized simulation caused $t_{0.5}^*$ to increase proportionally to $1/\gamma_{gb}$, independent of $\bar{f}_s$. For instance, Cases 4 and 7 were rescaled for $0.5\gamma_0$ and γ_0 , respectively, causing $t_{0.5}^*$ to decrease by a factor of 2.1. Similarly, the $t_{0.5}^*$ values for Cases 5 and 6 differed by a factor of 2.0. Rescaling a given simulation had no effect on n , as expected; Cases 4 and 7 both had $n = 2.06$ and Cases 5 and 6 had $n = 2.22$.

Increasing the grain boundary energy or average stored energy caused recrystallization to proceed faster, as shown in the plots in Figure 8 and the Avrami parameters in Table 2. Figure 8(a) shows the area fraction recrystallized vs. time for γ_{gb} values of $0.5\gamma_0$ (Case 4), γ_0 (Case 1), and $2\gamma_0$ (Case 5). The slope of the curve became steeper as γ_{gb} increased, corresponding to an increase in n from 2.06 to 2.22; $t_{0.5}^*$ decreased from 26.7 to 18.2 (Table 2). The changes to n and $t_{0.5}^*$ both caused recrystallization to occur faster for larger grain boundary energies. The recrystallization behavior was also simulated for stored energies of $0.5\bar{f}_{s,0}$ (Case 6), $\bar{f}_{s,0}$ (Case 1), and $2\bar{f}_{s,0}$ (Case 7), as shown in the simulated data in Figure 8(b). Increasing stored energy by a factor of four while fixing other parameters caused $t_{0.5}^*$ to drop from 36.5 (Case 6) to 13.0 (Case 7). This is a larger change than when the grain boundary energy alone is increased by the same factor, where $t_{0.5}^*$ decreased from 26.7 for Case 4 to 18.2 for Case 5. Additionally, n decreased from 2.22 to 2.06

when average stored energy was increased, in contrast to the increase in n for grain boundary energy. A decrease in n alone would slow recrystallization, but the faster recrystallization in Case 5 with respect to Case 4 is represented by the smaller value of $t_{0.5}^*$.

(a) Change grain boundary energy

(b) Change stored energy

Figure 8. Comparison of the area fraction recrystallized over time for five data sets (three simulations) employing different values of average stored energy or grain boundary energy. The reference data is Case 1 from Section 4.1 and employed the values of $\gamma_{gb} = \gamma_0$ and $\bar{f}_s = \bar{f}_{s,0}$; the values of γ_{gb} and $\bar{f}_s$ with respect to γ_0 and $\bar{f}_{s,0}$ are given in Table 2 for all data sets. For all cases, the simulated area fraction and the least-squares fit of the data to Eq. 19 are shown with data markers and lines, respectively. (a) Fraction recrystallized over time for three cases employing average stored energy of $\bar{f}_{s,0}$ and grain boundary energies of $0.5\gamma_0$, γ_0 , and $2\gamma_0$, identified in Table 2 as Cases 4, 1, and 5, respectively. (b) Fraction recrystallized over time for data sets with grain boundary energy of γ_0 and stored energies of $0.5\bar{f}_{s,0}$, $\bar{f}_{s,0}$, and $2\bar{f}_{s,0}$, denoted in Table 2 as Cases 6, 1, and 7, respectively.

6. Discussion

The relative contributions of stored energy and grain boundary energy can be estimated for the case of a single recrystallized grain in a polycrystalline deformed microstructure. The driving forces along a grain boundary are equivalent to pressures on the boundary and are related as [3]

$$\Delta P_{tot} = \Delta P_{gb} + \Delta P_s \quad (21)$$

where ΔP_{tot} is the total driving force, ΔP_{gb} is the driving force from grain boundaries, and ΔP_s is the driving force from stored energy. In this case, a positive driving force provides pressure for a recrystallized grain to grow within a polycrystalline deformed microstructure. The driving force exerted on the grain boundary of a particular grain within a polycrystalline microstructure can be estimated when the surrounding polycrystalline structure is viewed as a homogeneous medium over which grain boundary energy is distributed uniformly. The resulting expression is [42]

$$\Delta P_{gb} = c\gamma_{gb} \left(\frac{1}{\bar{r}} - \frac{1}{r} \right) \quad (22)$$

where r is the radius of the grain (a recrystallized grain in this particular case), $\bar{r}$ is the average grain size of the surrounding grains, and c is a geometric constant that depends on the dimensionality of grain growth ($c = 1/2$ in 2D and $c = 1$ in 3D [42], owing to the fact that the circular grain is effectively a cylinder in 3D). When considering recrystallization, the difference in stored energies between the particular recrystallized grain and its surroundings will also exert a driving force on the grain boundary. This can be estimated as [3]

$$\Delta P_s = \Delta f_s = \bar{f}_s \quad (23)$$

assuming that the stored energy of the recrystallized grain is zero and the surrounding deformed microstructure has uniform stored energy of value $\bar{f}_s$.

The driving forces can be quantified for the geometry of a single, round recrystallized grain in a polycrystalline deformed microstructure. This analysis uses the parameters for Cases 1-3: $r = r_{seed} = 7.5 \mu\text{m}$, $\bar{r} = D_{REX}/2 = 35 \mu\text{m}$, $\bar{f}_s = 5.3 \times 10^6 \text{ J/m}^3$, and $\gamma_{gb} = 0.7 \text{ J/m}^2$. Using Eqs. 22 and 23, $\Delta P_{gb} = -3.7 \times 10^4 \text{ J/m}^3$ and $\Delta P_s = 5.3 \times 10^6 \text{ J/m}^3$. Thus, the driving force from stored energy is estimated to be over two orders of magnitude larger than that of grain boundary energy. For simulations with a single deformed grain, the driving forces can be calculated using $\bar{r} = \infty$.

For the single-recrystallized-grain simulations described in Section 2.2.1, the large driving force from stored energy is expected to dominate microstructural evolution, as the ratio $|\Delta P_s/\Delta P_{gb}| \sim 140$ even at the initial stage where $r \sim r_{seed}$. The constant grain boundary velocities reported in Sections 4.1 and 4.2 are consistent with this observation.

Similar analyses can be performed to examine the relative importance of the driving forces for the parameters examined in Section 5, namely the initial deformed microstructure, stored energy, and grain boundary energy. According to Eqs. 21-23, ΔP_s is much larger than ΔP_{gb} . For example, the smallest $|\Delta P_s/\Delta P_{gb}|$ for the parametric study is 71 and hence the recrystallization kinetics is dominated by stored energy over grain boundary energy for all cases. Consequently, the average stored energy is expected to have a larger effect on kinetics than the underlying microstructure or grain boundary energy. We indeed observe this in the simulations. Specifically, different amounts of stored energy (Cases 1, 6 and 7) resulted in $t_{0.5}^*$ ranging from 13.0 to 36.5 and n ranging from 2.06 to 2.22; this was the widest variations in recrystallization kinetics observed in the parametric study, indicating the importance of stored energy in the systems examined. On the other hand, changing the grain boundary energy (Cases 1, 4, and 5) resulted in much smaller variations, namely $t_{0.5}^*$ ranging from 18.2 to 26.7 and n ranging from 2.06 to 2.22. The ranges of n for stored energy and grain boundary energy are identical since the same nondimensional simulations were used. Thus, the smaller range of $t_{0.5}^*$ for grain boundary energy indicates smaller variations in the overall recrystallization kinetics. Varying the initial microstructure in Cases 1-3 yielded even smaller variations, resulting in $t_{0.5}^*$ ranging from 20.7 to 23.3 and n ranging from 2.14 to 2.26 (Note that the variations for grain boundary energy may be overestimated due to the model artifact discussed below). Our results are also consistent with a previous study of two-grain phase field simulations by Moelans et al., which indicated that the amplitude of stored energy differences has a larger effect on grain boundary motion than both the length scale of these fluctuations or grain boundary energy [8]. Here, we quantify the sensitivity to grain boundary energy and average stored energy, S_{gb} and $S_{\bar{f}_s}$, respectively, as

$$S_{gb} = \frac{\Delta t_{0.5}^*/t_{0.5,0}^*}{\Delta \gamma_{gb}/\gamma_{gb,0}} \quad (24a)$$

$$S_{\bar{f}_s} = \frac{\Delta t_{0.5}^*/t_{0.5,0}^*}{\Delta \bar{f}_s/\bar{f}_{s,0}}. \quad (24b)$$

These calculate the change in $t_{0.5}^*$ with respect to γ_{gb} or $\bar{f}_s$ as determined using a linear least squares fit of the simulation parameter and corresponding $t_{0.5}^*$, where the numerators and denominators are normalized by reference values, denoted with a subscript 0. We calculate these to be -0.25 for grain boundary energy and -0.68 for stored energy using the results in Table 2 and taking Case 1 as the reference simulation. The larger magnitude of $S_{\bar{f}_s}$ as compared to S_{gb} indicates that a relative change to stored energy, such as doubling or halving the value, has a larger effect on $t_{0.5}^*$ as compared to a similar change to grain boundary energy. Nevertheless, it should be noted that, if the parameters are set such that the ratio $|\Delta P_s/\Delta P_{gb}|$ is more comparable, a change in grain boundary energy or the initial polycrystalline microstructure would be expected to alter the simulation results more significantly. Lastly, it is important to note that average stored energy is proportional to both average dislocation density and shear modulus (Eq. 1). Because the simulation results are sensitive to the average stored energy density, $\bar{\rho}$ and G should be carefully set to represent the physical system being simulated.

The predictions from driving forces (Eqs. 21-23) can be used to examine the accuracy of the simulated recrystallization kinetics. In Section 5.1, recrystallization was simulated with underlying microstructures of 174 and 1 deformed grain, denoted as Cases 2 and 3, respectively; $\bar{f}_s$ is held constant. The presence of grain boundaries in the deformed microstructure (Case 2) led to slightly faster recrystallization than a deformed microstructure with a single grain (Case 3). This is unexpected since Eqs. 22 and 23 predict that ΔP_{gb} should be about two orders of magnitude smaller than ΔP_s , and thus the underlying microstructure should have negligible effect on the kinetics. Similarly, increasing γ_{gb} resulted in faster simulated recrystallization (Section 5.2), despite ΔP_{gb} being negligible compared to ΔP_s . Furthermore, Eq. 22 predicts that ΔP_{gb} becomes more negative for larger γ_{gb} , which should slow down the recrystallization kinetics, directly contradicting the increased recrystallization kinetics observed in the simulation. Section 5.2 also investigated the effect of stored energy on recrystallization. In these simulations, increasing stored energy is correlated with faster recrystallization kinetics; this is consistent with the prediction that driving force increases with $\bar{f}_s$ (Eq. 23). The predictions in driving forces are in agreement with simulations that vary stored energy, but do not correlate to changes in the grain boundaries or grain

boundary energy. We examined the source of the discrepancy in detail and found it to originate primarily from spurious grain boundary energy effects, as described below.

To identify the origin of the unexpected effects from grain boundary energy, we compare the prescribed γ_{gb} to the calculated grain boundary energy ($\gamma_{gb,calc}$) that is determined from the values of the order parameters. We use the single-recrystallized-grain simulation described in section 2.2.1 and the corresponding results in sections 4.1 and 5.2. The order parameters of the recrystallized grain and deformed matrix are denoted by η_{rx} and η_{def} , respectively. For the forms of f_{bulk} and $f_{gradient}$ given by Eqs. 4 and 5, respectively, the grain boundary energy is calculated as [22]

$$\gamma_{gb,calc} = \int_{x_{center}}^{x_{edge}} \left\{ m_0 \left[\left(-\frac{1}{2} \eta_{rx}^2 + \frac{1}{4} \eta_{rx}^4 \right) + \left(-\frac{1}{2} \eta_{def}^2 + \frac{1}{4} \eta_{def}^4 \right) + \alpha \eta_{rx}^2 \eta_{def}^2 + \frac{1}{4} \right] + \frac{\kappa}{2} \left(|\nabla \eta_{rx}|^2 + |\nabla \eta_{def}|^2 \right) \right\} dx, \quad (25)$$

where the integration limits have been modified to span the x -axis from the center to the edge of the domain, x_{center} and x_{edge} , respectively; the grain boundary is at an intermediate location within the domain. This expression assumes that the stored and grain boundary energies are independent and that the curvature of the recrystallized grain has a negligible effect on $\gamma_{gb,calc}$. The results of these calculations are presented in Table 3. All three cases had larger $\gamma_{gb,calc}$ than the prescribed value; larger percent errors correspond to smaller γ_{gb} . Additionally, Figure 9 plots the order parameters near the grain boundary for the single-recrystallized-grain simulation with $\gamma_0 = 0.7 \text{ J/m}^2$ (Case 1) at $t_{corr}^* = 14.7$, where the center of the round grain corresponds to $x^* = 0$. The grain boundary is asymmetrical about the interface (located at approximately $x^* = 78$). Within a growing recrystallized grain (such as where $x^* < 78$), f_s is small and therefore in this region the evolution of the order parameter is controlled by γ_{gb} , whereas the deformed grain ($x^* > 78$) is dominated by $\bar{f}_s$. The asymmetrical profile causes $f_{gradient}$ to be artificially enhanced within the recrystallized grain. This effect is largest for simulations with small γ_{gb} , causing simulated recrystallization to proceed slower, leading to the unexpected behavior observed in Case 4 as compared to Case 5. The result indicates that the present phase field model of recrystallization should be applied with care to avoid drawing conclusions upon spurious results, and improvement

should be considered in order to eliminate these spurious effects in the model. Furthermore, other phase field recrystallization models should be evaluated for these spurious effects.

Table 3. Nominal and calculated grain boundary energies, γ_{gb} and $\gamma_{gb,calc}$, respectively, for the single-recrystallized-grain simulations for Cases 4, 1, and 5 from Section 5.2. The percentage error between the values is listed.

	γ_{gb} (J/m ²)	$\gamma_{gb,calc}$ (J/m ²)	Error
Case 4	$0.5\gamma_0 = 0.35$	0.41	17%
Case 1	$\gamma_0 = 0.7$	0.77	10%
Case 5	$2\gamma_0 = 1.4$	1.44	3%

Figure 9. Plot of the order parameters near the grain boundary for the two-grain simulation with $\gamma_{gb} = \gamma_0 = 0.7 \text{ J/m}^2$ (Case 1) at $t_{corr}^* = 14.7$. The order parameters η_{def} (for the deformed grain) and η_{rx} (for the recrystallized grain) are marked with * and o markers, respectively; adjacent values are connected with straight lines for visualization.

Finally, we note that the Avrami exponents for Cases 1-7 are consistently larger than the theoretical value of two because of the specific set of initial positions of the recrystallized grains. The initial nuclei locations in Case 1 were selected stochastically and resulted in $n = 2.15$; different random nuclei locations (Section 4.1) yielded n between 1.87 and 2.15. The set of nucleus positions used in Case 1 (selected as the baseline case in this study) happened to have the largest n among the six simulations in Section 4.1. Since all simulations share the same nuclei positions as the baseline Case 1, which had an enhanced value of n , it is not surprising that the all simulations

yielded n greater than the theoretical values of 2, and the values of n are likely over-estimated by ~10%.

7. Summary and Conclusions

In this paper, we presented a phase field model and validate it for static recrystallization. The initialized recrystallization microstructure was generated by seeding grains on an underlying polycrystalline microstructure. A stochastic method was utilized to determine locations at which circular or spherical dislocation-free grains were seeded. The nuclei were preferentially placed on grain boundaries and triple junctions of the initial microstructure such that none were placed in the interior of grains. Growth of a single recrystallized grain was simulated to estimate the time required for a nucleus to grow from its critical size to its seeded size. Based on this estimate, a correction to the simulation time was obtained to account for the time associated with the initialization of the recrystallized grain. The recrystallization phase field model was implemented for parallel processing utilizing MPI so that large, 3D microstructures may be simulated employing high-performance-computing resources.

Simulations were performed in two and three dimensions for comparison to theoretical Avrami kinetics. With the time corrections, the Avrami exponents were found to be 2.00 ± 0.11 and 3.12 for two and three dimensions, respectively, which are in agreement with the Avrami model for site-saturated nucleation. Furthermore, the Avrami parameters changed significantly when time corrections were included, indicating the corrections are necessary for accurate characterization of recrystallization kinetics.

We also investigated the sensitivity of the simulation results to the initial microstructure, stored energy, and grain boundary energy. We provided an estimate of the relative contributions from the stored energy and the grain boundary energy to the driving force for recrystallization for the parameter set chosen. The driving force was shown to be dominated by the stored energy, which was consistent with the simulation results that exhibited higher sensitivity to the change in stored energy than grain boundary energy. Increasing or decreasing average stored energy by a factor of two resulted in larger variations in the recrystallization kinetics than similar changes to grain boundary energy. The effects of stored energy and grain boundary energy on the recrystallization kinetics were larger than the variations caused by different initial microstructures. When grain boundary energy is small, a spurious effect was observed due to the change in the

order parameter profile and resulting error in the actual grain boundary energy (ranging from a few percent up to 17% for the parameter sets examined in this work). Such diffuse interface effects can significantly affect the results in some cases, and thus the phase field model should be applied with care and be improved to eliminate such effects in the long term.

The recrystallization phase field model described here holds promise to simulate microstructural evolution in specific material systems, such as titanium and magnesium alloys, when parameterized accordingly. Additionally, it provides the modeling framework for further studies of complex recrystallization phenomena. For example, experiments have observed necklace formation, whereby several recrystallized grains form adjacently on a grain boundary [3]. The nucleation scheme could be modified to prefer nucleation close to other nuclei or in highly deformed regions of the microstructure to examine the effect of nucleation sites. Furthermore, the model is extendable to include additional microscale physics, such as anisotropic grain boundary energy [43], to examine other phenomena like texture evolution. Detailed simulations are important for complicated recrystallization scenarios that may not be fully described by a simple analytical model. Additionally, three-dimensional simulations can be directly compared with experimental data for validation. Finally, we note that the model contributes to the developing software infrastructure, which would provide not only the mechanistic understanding of microstructural evolution but also the linkage needed for integrating models across Integrated Computational Materials Engineering (ICME) tools. For example, the simulated microstructures can be passed to microstructure-level mechanical behavior simulations [44] within an ICME framework.

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Research Data

The processed data required to reproduce these findings are published on Materials Commons and available to download from Ref. [45].

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