EFFECTS OF GRAIN BOUNDARY CHARACTER ON DYNAMIC RECRYSTALLIZATION USING A MODIFIED MONTE CARLO METHOD

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ABSTRACT

Effects of Grain Boundary Character on Dynamic Recrystallization Using a Modified Monte Carlo Method

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Dynamic recrystallization (DRX) is the recrystallization that occurs during high temperature deformation of metals and alloys. While DRX has been observed experimentally, the parameters that affect the microstructure are still being explored. For example, the effects of temperature, strain rate, and initial grain size have already been studied, yet the effect of initial special boundary fraction is still unknown. Special boundaries are high-angle, low-energy grain boundaries. It is believed that higher initial fractions of special boundaries will lead to a delay in the onset of recrystallization and a higher peak stress.

Experimentation has shown that triple junctions are preferred nucleation locations for DRX. This work will look at the different types of triple junctions (categorized based on the number of special boundaries at the junction) and determine the effect that special boundaries have on the probability of nucleation. It was supposed that triple junctions without special boundaries would be preferred nucleation sites due to higher grain boundary energy. This work showed that triple junctions sites, particularly triple junctions without special boundaries, were the preferred nucleation location.
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1 INTRODUCTION

1.1 Motivation for Research

Dynamic recrystallization (DRX) involves grain growth and simultaneous recrystallization during high-temperature deformation in materials with low stacking fault energies. Prior to 1965, recrystallization was thought to be a process where the grain refinement and reduced strain hardening occurred after processing and during annealing only [1]. However, as material characterization techniques improved, it was seen that at certain temperatures and strain rates, grain growth, recrystallization, and an overall reduction of strain hardening occurred during high-temperature material processing and can alter a material’s microstructure. This observation, combined with the discovery that microstructure plays an important role in macroscopic material properties, gave rise to the study of recrystallization during processing, called dynamic recrystallization.

By improving our understanding of DRX, it may be possible to tailor processes and materials to more precisely suit specific applications. This understanding can be aided through the development of realistic simulations of the DRX process. Developing a simulation requires mathematical equations that reflect the physical processes of DRX. This simulation provides a possible outcome that can be validated by applying the same experimental parameters to the material from which the initial microstructure was obtained. Imaging the material after physical experimentation can help to validate the observations derived from the simulation.

By comparing the simulated results with experimental results, it is possible to continue to build on the developed computer program to allow accurate DRX simulation for materials beyond those used for this thesis. While the goal of this thesis is to complete the objectives listed in the
next section, the implications extend far beyond them, allowing additional investigation into DRX in materials other than stainless steel 316L and nickel.

1.2 Objectives

In the 1980s, the Monte Carlo method was adapted to examine the mechanics of grain growth and nucleation. This method involved converting a sample area into discrete sites that could then be selected at random and algorithms were then applied to simulate specific processes [1, 2]. For this thesis, a modified Q-state Potts model was chosen to simulate DRX using experimentally obtained microstructures [3].

Built off previous work at Boise State University, the first objective of this thesis was for the simulation to accept data from experimental EBSD scans and use the information as a starting point for each run. Multiple strains and nucleation rates were simulated and various parameters affecting the kinetics of DRX were explored: specifically, initial special boundary fractions and initial grain size. Finally, specific simulation parameters were determined that produced simulated results similar to the physical results in the materials that were utilized in congruent experiments. Also, the effect of a sample’s initial special boundary fraction is of particular interest as it is hypothesized that the kinetics of DRX is affected by the fraction of boundaries that are considered high-angle yet have lower boundary energies than is typically expected for a high-angle boundary. A boundary’s energy is thought to be a leading cause as to whether or not a nucleus forms at that location. This thesis aims to include varying grain boundary energies, with specific interest in low-energy boundaries, to design an energy-driven simulation that simulates DRX based on current theories derived from experimentation.
2 BACKGROUND INFORMATION

Dynamic recrystallization involves a combination of grain growth and simultaneous recrystallization during high-temperature deformation of metals and alloys. This occurs when a material with an average low- to medium-stacking fault energy is heated to approximately half its melting temperature while being strained in compression, tension, or torsion [1, 4–7]. Recrystallization has been described by R.D. Doherty et al. [1] as the formation of new grains due to the mobility and formation of high-angle boundaries. During DRX, the explanation for the experimentally observed recrystallization and grain growth is reduction of strain energy [8].

In order to build a computer program to simulate DRX, experimental observations must be incorporated in a model that statistically represents the behavior observed in DRX experiments. The program developed for this thesis is based on a modified Monte Carlo Q-State Potts model [3]. This model provides a randomized approach and allows for a purely energy-driven simulation. As with any model, the mechanics and kinetics of a particular process must be understood and converted to mathematical equations; this is no different for DRX.

2.1 Grain Boundary Types and Classification

Dislocations are defects at particular sites where the regular crystal structure is interrupted. The study of dislocations has resulted in a realization that the number and placement of these atomic defects affects the larger scale characteristics of materials. One contribution of dislocation theory to DRX research is the idea that grain boundary energy is independent of grain size [9]. This is because the energy along a boundary does not extend more than a limited distance into the grain, meaning that boundary energy is dependent on material properties and misorientation.
between grains rather than on grain size. It has recently been proposed that grain boundary planes have a significant effect on grain boundary energy [10]. The inclusion of planes in this simulation has been neglected, however, in order to develop a starting point on which additional parameters can be added at a later date.

As the dislocation density increases during straining, nuclei are able to form during deformation [6]. Once recrystallization begins, dislocations in the material are eliminated. When the dislocation density gets low enough, recrystallization is halted until the strain increases the density to a critical amount [6]. This increase, and subsequent decrease, in dislocations only occurs in materials with low- to medium-stacking fault energy that undergo deformation at temperatures near half of their melting points [1]. If a material with high-stacking fault energy undergoes the same heating and deformation process, the dislocations in the material are eliminated in pairs, which leads to steady state flow. This behavior in high-stacking fault materials is known as “dynamic recovery,” or DRV. A comparison of DRX and DRV is shown in Figure 2.1. The transition from linear hardworking to perfectly plastic flow occurs in the DRV region of the figure. Once the slope of the stress-strain curve begins to decline, the curve enters the DRX region.

Measurements of grain boundary energy have shown that there are particular grain boundary misorientations that result in lower grain boundary energy [12]. These low-energy, high-angle boundaries have become known as “special boundaries.” The boundaries are considered special as they deviate from the previous assumption that higher grain misorientation directly implied that the grain boundary energy; this was mostly due to what was modelled by Read and Shockley who showed increasing dislocation content until a misorientation of 20° [13]. Grain boundary energy for misorientations higher than 20° were observed to be constant [14]. However, it appeared that certain high-angle boundaries had lower grain boundary energies and consequently could be modeled instead as low-angle boundaries [9]. These special boundaries have been cat-
Figure 2.1: Dynamic recovery is evident by a non-linear stress-strain curve while dynamic recrystallization results in a curve with a portion of the curve having a non-positive slope. Modified from [11].

categorized by the inverse number of coincident sites. For example, a Σ3 boundary has \( \frac{1}{3} \) of total lattice sites are coincident.

A number of the grain boundary misorientations corresponding to grain boundary energy minima have been identified as having a large number of coincident sites. Coincident sites occur when certain atomic positions from neighboring grains overlap and “share” a single atom [15]. The densities of coincident sites have been given Σ classifications and the number following the Σ designation is the inverse of the number of overlapping lattice sites [1]. In order to simplify the essentially infinite number of boundary combinations, a discrete number of ideal Σ classifications have been determined and for the purpose of this thesis, only six designations (Σ1, Σ3, Σ9, Σ11, Σ27a, and Σ27b) will be taken into account. Any higher Σ classifications will simply be considered as a “general boundary.” To simplify the calculations required to simulate DRX, the Brandon criterion [12] was used to group the number of boundary interfaces into discrete.
boundary classifications. Brandon hypothesized that a boundary that deviates from the ideal CSL angle could be considered ideal if the misorientation was close to the ideal angle.

The Brandon criterion was developed based on the concept that CSL boundaries are able to be approximated as ideal CSLs as long as the boundary’s misorientation is within a specified number of degrees of the ideal CSL. For high densities of coincident sites (i.e., low Σ values), the degree of deviation from an ideal CSL is greater than for boundaries with higher Σ values. Multiple variations of this criterion have been provided that are more conservative (i.e., Palumbo-Aust criterion), but for the purpose of this thesis, the Brandon criterion was selected. Using a criterion to simplify the possibly infinite misorientations into a discrete number of categories simplifies the calculations necessary to categorize grain boundaries. Brandon’s equation for the allowable angle of deviation, Δθ_{max}, is as follows:

\[ Δθ_{max} = θ_0Σ^{-1/2} \]  \hspace{1cm} (2.1)

where θ₀ is agreed to be 15° and Σ is the CSL type (3 for a Σ3, etc.).

The widely accepted definition for a “high-angle boundary” is a boundary with a misorientation of greater than 15° [12, 15]. In this study, in order to simplify the classification of essentially an infinite number of combinations of grain boundary interfaces, a method was designed to specify the maximum variation of a boundary’s misorientation angle from a coincident site lattice (CSL). A CSL boundary is given a “sigma” designation, which is the inverse of the number of overlapping lattice sites [16]. For example, a Σ3 boundary type would have one-third of the lattice sites overlapping. In contrast to a “high-angle” boundary, a “low-angle” boundary is considered to be an interface where the angular misorientation is less than 15°. Generally a
low-angle boundary will have significantly less boundary energy than a high-angle boundary but special high-angle boundaries exist with uncharacteristically low-boundary energy.

It has been shown [12, 15] that certain misorientations and grain boundary plane combinations result in lower grain boundary energy than would be expected for high-angle boundaries [9]. As shown in Figure 2.2, certain high-angle boundaries (those with misorientation angles of greater than 15°) have a lower energy than others. These high-angle, low-energy boundaries occur when a boundary is said to have coincidence, which is essentially when two grains have a high degree of fit (see Figure 2.3). A boundary has high coincidence when the density of overlapping lattice sites is high. When a boundary has low coincidence, the lattice sites that do not overlap are terminated in a dislocation. The number of these dislocations and their placement determines the amount of energy associated with the boundary, as described by Read and Shockley’s dislocation model for low-angle and coincidence site lattice boundaries [9]. For general high-angle boundaries, the dislocation content is such that it is difficult to describe as an orderly array of dislocations.

**Figure 2.2:** Experimental plot of grain boundary energy as a function of misorientation for <110> plane in Aluminum. High-angle boundaries with lower energy are considered “special” while other high-angle boundaries are considered “general.” Modified from [17].
2.2 Strain and Stored Energy

Strain energy is the driving force for two processes in DRX, grain growth and recrystallization [8], and so it is prudent to include strain in any simulation that models DRX. In our simulations, strain energy is applied at a constant rate and stored in each tile in the simulative lattice. During DRX, two different methods take place to reduce both the stored energy and grain boundary energy in each tile, and therefore reduce the energy in the entire system.

At the onset of straining, while stored energy is still relatively low, the system energy is reduced through grain growth (thereby reducing the contribution from grain boundary energy). As the stored energy begins to increase to a point where grain growth is no longer an efficient energy reduction method, recrystallization begins. By nucleating strain-free grains, recrystallization effectively begins to lower the overall energy until the energy associated with boundaries formed by nucleation outweighs the benefit of reducing the stored energy. This grain growth/recrystallization cycle continues until the average stored energy achieves steady state. This transition between grain growth and recrystallization portions of DRX that results in the cyclic behavior shown in Figure 2.4. While the axes on the figure specify “Average Stored Energy” vs. “Monte Carlo Steps,” this behavior can also be seen in experimental stress-strain curves.
2.3 Recrystallization

Recrystallization is the formation of new grains, or nuclei. This thesis deals specifically with recrystallization that occurs during thermo-mechanical processing. It is important to recognize that recrystallization occurs both dynamically (DRX) and statically (SRX). The difference between them is when the recrystallization occurs. SRX was observed prior to DRX and it was not until the 1960s that the difference between the two types of recrystallization was established [18]. Advancements in material characterization techniques were required in order to make the following distinctions: recrystallization during processing (which is considered DRX) and recrystallization after processing (which is considered SRX).

It is important to make a distinction between thermal recrystallization that occurs during solidification and DRX. When comparing the predicted rate of formation of new grains predicted by the dominant kinetic model of nucleation model to the observed rate during DRX, the observed rate was found to be significantly larger [1]. The thermal fluctuation model has been successfully applied to solidification and is therefore found to be a valid model for certain applications [1].
Since the deviation in the observed nucleation rate, which was on the order of $10^{50}$ times larger than predicted, it is possible to state that the method of recrystallization during DRX is not the same as that which has been found in solidification and phase transformations.

Once DRX was identified, further studies were required to examine the behavior of recrystallization during DRX. The nuclei that form during DRX have been observed to be free of strain energy when they are initially formed [1, 19]. Proposed in 1949 by Cahn [20] using XRD and more recently supported by SEM results [21], an understanding has been established that nucleation is not the formation of an entirely new grain, but rather a separation of portions of existing grains. This separation occurs after a grain boundary becomes serrated and additional strain causes grain boundary shearing, which separates the serrated portion and resulting rotation leads to the formation of a new grain (see Figure 2.5) [22, 23]. While this is one possible method of recrystallization, the exact mechanism of recrystallization is still unknown.

Experimental results show a number of preferences for nucleation during DRX. First, nuclei form “necklace” structures by nucleating along existing grain boundaries [23]. However, the most preferential nucleation location has been identified by Miura et al. as triple junctions, specifically at triple junctions with high-angle boundaries [8]. The nuclei that form at triple junctions have also been observed to form $\Sigma 3$ boundaries with a neighboring grain [8].

2.4 Conditions of Dynamic Recrystallization

Temperature, strain rate, and grain size are all factors that have been shown experimentally [4, 5, 24, 25] to have an effect on DRX. The effects of temperature and strain rate were examined by Petkovic et al. [11] using 0.68% C steel (Figure 2.6). Petkovic et al.’s results showed that the conditions that encourage dynamic recrystallization are small strain rates, and high temperatures. Higher temperature increases both the grain growth and recrystallization rates.
(a) Boundary corrugation accompanied by the evolution of subboundaries.

(b) Partial grain boundary shearing, leading to the development of inhomogeneous local strains.

(c) Bulging out of a serrated grain boundary and the evolution of strain induced subboundaries due to grain boundary shearing and/or grain rotation, leading to the formation of a new DRX grain.

**Figure 2.5:** A schematic modified model for the nucleation of a grain at a grain boundary (GB) [22].

**Figure 2.6:** Experimental stress-strain curve for 0.68 % C steel. Image adapted from [11].
The rate of DRX has been described by the Zener-Holloman parameter as follows:

$$Z = \dot{\varepsilon} \exp \left( \frac{-Q}{RT} \right)$$  \hspace{1cm} (2.2)

where $\dot{\varepsilon}$ is the strain rate, $Q$ is the apparent activation energy for deformation, $R$ is the gas constant, and $T$ is the temperature. By this definition, a high $Z$ value would describe conditions that are not favorable to DRX (high strain rate and low temperature), while one may be more likely to observe DRX under low $Z$ conditions. The correlation of $Z$ value and DRX behavior has been explored by Sakai and Jonas [6] with initial grain size. For example, a system with a low $Z$ value and a low initial grain size is likely to exhibit multiple peak behavior while a low $Z$ and a high initial grain size will be more likely to exhibit single peak behavior.

### 2.5 Kinetics of Dynamic Recrystallization

Besides exploring the mechanics of DRX, the rates of grain growth and nucleation are also of interest. One factor that affects the rate of recrystallization is grain size. Wahabi et al. [5] approached the kinetics of DRX by hypothesizing that the number of available nucleation sites directly relates to the kinetics of DRX. As nucleation occurs, the number of available sites decreases; this point determines when the curve shown in Figure 2.4 returns to an upward slope. Experimentally, samples with smaller grain sizes have been observed to begin DRX earlier than samples with larger grains due to an abundance of grain boundaries on which nuclei can form while samples with larger grains experience a delay (during which stored energy, $H$, continues to increase) before beginning to nucleate [5].

The Johnson-Mehl-Arram (JMA) formula [26] is a method of tracking the progress of recrystallization. The formula describes the volume fraction of transformed volume (i.e., fraction
of volume that has recrystallized) as:

\[
\frac{dV_t}{dV_{ex}} = (1 - V_t)
\]  

(2.3)

where \(V_t\) is the transformed volume (volume of recrystallized grains) and \(V_{ex}\) is the extended volume (total volume of sample). Plotting the volume fraction of recrystallized material is useful for analyzing DRX as the rate of recrystallization and the time at which DRX starts can quantify the effect of various parameters on DRX.

The effect of initial grain size was explored further by Wahabi et al. [5] as a factor that affects the kinetics of DRX. Wahabi et al. demonstrated that microstructures with small initial average grain sizes recrystallized earlier than samples with larger initial average grain sizes. The reasoning behind this behavior was that samples with smaller grain sizes have a larger volume fraction of grain boundaries and therefore a higher number of available nucleation sites. This result supported the modified JMA equation for DRX kinetics, which includes an initial grain boundary term [6]:

\[
X = 1 - \exp\left\{-\frac{K}{D_0}t^n\right\}
\]  

(2.4)

where \(X\) is the volume fraction of recrystallized material, \(K\) and \(n\) are constants, \(D_0\) is the initial average grain size, and \(t\) is time. This equation shows that the rate of recrystallization is slower for larger initial grain size.

While the effect of initial special boundary fraction on the rate of recrystallization is still uncertain, this thesis looks to explore this relationship and show a relationship between the two. However, due to the inhibiting effect special boundaries have on nucleation due to their resistance to grain boundary sliding [8], it stands to reason that materials with a higher percentage of these
high-angle, low-energy boundaries would also experience a delay in the onset of recrystallization similar to the delay observed in large grain samples. Experimentation has also shown [8] that while nucleation is preferred at triple junctions, triple junctions with twin boundaries (Σ3 boundaries) are much less preferred than triple junctions without twin boundaries.

### 2.6 Monte Carlo Simulation

Monte Carlo simulation uses random sampling to choose a site, then applies algorithms to reduce the energy in a system. Depending on the Hamiltonian associated with the system being simulated, the energy terms will continue to decrease each Monte Carlo step until steady state is attained. A “Monte Carlo step” is proportional to time. For any single step, a number of test sites are selected where the number of selections is equal to the number of discrete test sites present in the system.

First developed by Metropolis and Ulam [2], the Monte Carlo method was designed for applications related to quantum physics. However, the applications now stretch beyond those for which it was first developed [27, 28]. As stated in Section 1.2, Monte Carlo was found to be a suitable algorithm to simulate grain structure evolution [19]. Since that time, a number of modified Monte Carlo methods have been developed [3]. The method used in this thesis deals with a Monte Carlo Potts Model, similar to what was used by Rollett et al. [29] and Peczak and Luton [30].

The Q-State Potts model [3] was used as the basis of this work. The $Q$ in “Q-state” implies that the tiles in the lattice can have $Q$ different states [3]; in the particular application of simulating DRX, a system can have $Q$ different grains. The value for $Q$ in our work is essentially infinite since the simulation allows the introduction of new grain orientations rather than retaining the same number of grains present in the initial microstructure.
Tile shape also plays an important role in the lattice behavior. The lattice used is described as a triangular lattice with a hexagonal Wulff shape (Figure 2.7). As discussed by Rollett, a triangular lattice is suitable for 2D applications as its geometry does not inhibit grain growth [27].

![Figure 2.7](image)

**Figure 2.7:** Each hexagon represents an individual sample site. The varying colors represent the orientation of the particular tiles and similar orientations are grouped into grains and neighboring grains are separated by a grain boundary, noted here by a thick black line.

The method for choosing sample locations on which to apply DRX algorithms involves assigning a number to each tile in the EBSD scan and then randomly generating a number between 1 and the total number of tiles present and selecting the tile corresponding to the chosen number. Once a tile has been chosen, one of two different types of calculations are performed: to determine whether or not the chosen tiles will recrystallize or to determine if the grain in which the tile is contained will grow. Equations for recrystallization and grain growth, and additional details on the simulation method, are discussed in detail in the following chapter.
3 SIMULATION PROCEDURES

An earlier version of the code used for this work [31] was assembled using Visual Basic and Microsoft Excel. In order to make the code more universal (i.e., less dependent on a particular program and operating system) and to decrease computation time, the code was converted into ANSI C programming language.

Building an energy-based simulation requires energy equations to which minimization techniques can be applied. The inputs to the simulation consist of individual tiles that are grouped into grains based on similar orientations. An effort to reduce the overall system energy must then require the energy associated with individual tiles to be minimized.

While the boundary energy is important to simulate DRX, it is the value of the stored energy in the entire system that provides the most useful insights into the behavior of the simulation. Figure 2.4 is a plot of the average stored energy as a function of the Monte Carlo steps. A positive slope indicates that grain growth is the dominant process; when the curve has a negative slope, recrystallization is the dominant process and strain free grains are being created.

The cyclic stress-strain behavior (and subsequent decrease in this behavior with decreasing temperature or increasing strain rate) is key to identifying DRX in experimental work and should be evident in DRX simulations. Other works [5, 27] have used the average stored energy per tile as a function of Monte Carlo steps to produce graphics that allow the same cyclic behavior to be observed in simulations. This same method was used in this thesis to produce plots comparable to the stress-strain plots obtained from experimental results.
After a fixed number of Monte Carlo steps, the simulation totals the stored energy present in every tile. Dividing the total stored energy by the total number of tiles produces the average stored energy per tile (Eq. (3.1)):

\[ H_{\text{avg}} = \frac{H_{\text{total}}}{n} \]  

(3.1)

where \( H_{\text{avg}} \) is the average stored energy, \( H_{\text{total}} \) is the sum of all the stored energy in all tiles, and \( n \) is the total number of tiles.

3.1 Overview of Simulation Process

This research simulates DRX by performing a prescribed number of Monte Carlo steps. The program first counts the number of tiles present in the initial microstructure and that value is stored as the number of tiles that must be chosen at random each Monte Carlo step (MCS). While the algorithm for grain growth is allowed to occur every time a tile is selected, the recrystallization algorithm is only applied until a number of specified new grains are formed. Once a specific number (determined by the nucleation rate) of grains have been formed in a particular MCS, the recrystallization algorithm will be skipped until the next MCS. Also, at the beginning of each MCS, a fixed value is added to the stored energy value of each tile to simulate the continual deformation that occurs to produce DRX. The exact value that is added depends on the strain rate being simulated. For example, a smaller strain rate would add less stored energy per MCS than a larger strain rate. This process, illustrated schematically in Figure 3.1, repeats until the specified number of Monte Carlo steps have been performed.

3.2 Grain Boundary Classification

One of the key differences between the current simulation and previous work done is the ability of this program to model anisotropic grain boundary energies. The method used to assign
Figure 3.1: A flowchart showing the general concept of what occurs during the simulation. The dashed line represents what operations are performed each Monte Carlo step.

The energy of a boundary is based on the misorientation between two grains. The misorientation can be described as the transformation necessary to rotate the normal vector of one grain onto that of its neighbor. Before the misorientation can be calculated, an orientation matrix for each grain must be determined as:

\[
g_x = \begin{pmatrix}
g_{11} & g_{12} & g_{13} \\
g_{21} & g_{22} & g_{23} \\
g_{31} & g_{32} & g_{33}
\end{pmatrix}
\]  

(3.2)
where $g_x$ is the orientation matrix, the subscript $x$ denotes a specific grain, and each element of the matrix is described as:

\[
\begin{align*}
g_{11} &= \cos(\phi_1) \cos(\phi_1) - \sin(\phi_1) \sin(\phi_2) \cos(\Phi) \\
g_{12} &= \sin(\phi_1) \cos(\phi_2) - \cos(\phi_1) \sin(\phi_2) \cos(\Phi) \\
g_{13} &= \sin(\phi_2) \sin(\Phi) \\
g_{21} &= -\cos(\phi_1) \sin(\phi_2) - \sin(\phi_1) \cos(\phi_2) \cos(\Phi) \\
g_{22} &= -\sin(\phi_1) \sin(\phi_2) - \cos(\phi_1) \cos(\phi_2) \cos(\Phi) \\
g_{23} &= \cos(\phi_2) \sin(\Phi) \\
g_{31} &= \sin(\phi_1) \sin(\Phi) \\
g_{32} &= -\cos(\phi_1) \sin(\Phi) \\
g_{33} &= \cos(\Phi)
\end{align*}
\]

where $\phi_1$, $\phi_2$, and $\Phi$ are the Euler angles for a grain and used to describe the deviation from the coordinate system used during EBSD scanning.

For the purpose of simplicity, only two grains will be considered during these calculations, grain A and grain B. Therefore, each grain will have an orientation matrix: $g_A$ and $g_B$. After an orientation matrix for each grain has been developed, the misorientation between grains A and B, $\Delta g_{AB}$, can be determined as:

\[
\Delta g_{AB} = g_A g_B^{-1}
\]  (3.3)
Once the misorientation matrix \((\Delta g_{AB})\) has been determined, it is multiplied by the 24 possible rotations for a cubic crystal structure to determine the minimum rotation necessary to rotate grain A onto grain B. The minimum rotation angle, \(\theta_{AB}\), is determined by:

\[
\theta_{AB} = \cos^{-1}\left( \frac{\sum_{i=1}^{3} a_{ii} - 1}{2} \right)
\]

(3.4)

where \(a_{ii}\) represents the diagonal elements of \(\Delta g_{AB} \cdot R\) with \(R\) being one of the 24 possible rotation matrices (each rotation matrix represents rotation about a different rotation axis). In short, the rotation matrix that results in the largest trace is the rotation operation that rotates grain A to match the orientation of grain B with the smallest angle of rotation. The result of multiplying \(\Delta g_{AB}\) by the rotation matrix, which results in the lowest angle of rotation, \(R_{min}\), is then compared to the 24 possible rotation matrices using the equation:

\[
\Delta \theta = (\Delta g_{AB} \cdot R_{min}) \cdot A_{CSL}^{-1}
\]

(3.5)

where \(\Delta \theta\) is the angular deviation of the misorientation from an ideal CSL boundary and \(A_{CSL}\) is the matrix used to describe each ideal CSL boundary. The \(\Delta \theta\) matrix that results in the largest trace (i.e., the smallest angle) then determines the CSL to which the boundary between grains A and B is closest. A final step in the boundary characterization process is to compare the resulting angle from \(\Delta \theta_{min}\) to the maximum deviation specified by the Brandon criterion for the corresponding CSL. If the angle is within the boundaries set by the Brandon criterion, the boundary is then approximated as being an ideal CSL boundary. If \(\Delta \theta\) is outside of the values specified by the Brandon criterion, then the boundary is assumed to be a general, or “high-angle,” boundary. The value of energy assigned to each CSL is a percentage of energy in relation to the
energy of a general boundary, which was obtained experimentally. For example, the energy of a general boundary in 304 stainless steel is 835 mJ·m$^{-2}$ and the energy of a coherent twin boundary ($\Sigma 3$) is 19 mJ·m$^{-2}$, or 5% of the energy of a general boundary [17]. Therefore, the simulation assigns an energy of 1.0 (or 100%) to a boundary found to be general and 0.05 (or 5%) to a $\Sigma 3$ boundary. Other $\Sigma$ boundaries were assigned energies between 0.05 and 0.65 as the particular energies of these boundaries were not the primary focus of this work. A summary of the grain boundary energies used for this work can be found in Table 3.1. The energy value for $\Sigma 1$ boundaries was assigned by approximating the energy equation

**Table 3.1:** A list of the grain boundaries that are taken into account by the simulation and their assigned energy values.

<table>
<thead>
<tr>
<th>Boundary Type</th>
<th>Simulated Energy Value ($H$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Sigma 1$</td>
<td>$\frac{\theta}{15}$</td>
</tr>
<tr>
<td>$\Sigma 3$</td>
<td>0.05</td>
</tr>
<tr>
<td>$\Sigma 9$</td>
<td>0.5</td>
</tr>
<tr>
<td>$\Sigma 27$</td>
<td>0.65</td>
</tr>
<tr>
<td>High-angle boundary</td>
<td>1.0</td>
</tr>
</tbody>
</table>

Classifying boundaries as special and general not only allows anisotropic simulation, but also allows an accurate method to calculate the fraction of boundaries in the system according to their CSL designation. When calculating the special boundary fractions, the simulation determines the fraction of special and general boundaries both by length and by number. Further on in each iteration, the program then differentiates between low-angle boundaries, $\Sigma 3$, $\Sigma 9$, $\Sigma 27$, and general high-angle boundaries. A boundary is considered “low-angle” if it has a misorientation angle of less than 15° while a high-angle boundary is any boundary with a misorientation angle greater than 15°, which does not have a $\Sigma$ classification.
Figure 3.2: (a) Shows a triple junction with no special boundaries present, (b) with a single special boundary, (c) with two special boundaries, and (d) with three special boundaries.

In order to validate the results of the simulation, the special boundary fractions of experimentally obtained EBSD scans being reported by the simulation were compared to the fractions reported by commercially obtained software TSL OIM Analysis 5. The results from this comparison resulted in a restriction being placed on the minimum misorientation angle between two tiles in order to determine if a boundary exists or not. This has the largest effect on the number of $\Sigma 1$ boundaries reported by the output files of the simulation and the TSL software. This minimum misorientation requirement prevents an unusually large number of $\Sigma 1$ boundaries from being reported and shown on the figures produced by the TSL software. For the purpose of this simulation, tiles with a misorientation of less than four degrees are considered to be the same grain and therefore not be separated by a boundary.

Another component of grain boundary classification is the ability to categorize triple junctions based on the number of special boundaries present at a junction. Tracking the number of triple junctions present in the sample throughout the simulation then was an objective of this thesis. Therefore, a method of tracking nucleation formation was introduced. The simulation categorizes triple junction sites as “$J$” types. For example, a “$J0$” location is a location in which there are no special boundaries present at the triple junction site, whereas a “$J3$” location would be a triple junction where there would be three special boundaries present (see Figure 3.2).
3.3 Dynamic Recrystallization

For a purely energy driven simulation, the decision of whether or not to nucleate a grain depends on the current energy at a test site and what the energy would be should a nucleus form. The energy difference between the proposed and existing tiles must be less than the energy required to form a new grain in order for nucleation to occur. The following relationship was used as a decision-making criteria of whether or not to nucleate a new grain:

\[
\text{Nucleate if: } \Delta \gamma + \Delta H + E_{\text{form}} \leq 0
\] (3.6)

where \( \Delta \gamma \) was the change in grain boundary energy, \( \Delta H \) is the change in stored energy, and \( E_{\text{form}} \) is the energy required form a new grain. The value of \( E_{\text{form}} \) was considered a variable and can be altered in order to allow future accommodation of various materials. Physically, \( E_{\text{form}} \) corresponds to the energy required for a portion of an atomic lattice to break its bonds with a parent grain and reorient to a new grain. It was assumed that each material may require a different amount of stored energy that is required to cause recrystallization.

The process of nucleating a new grain was done by choosing a tile randomly along with two of its neighboring tiles. The grain boundary energy and stored energy of the three selected tiles were calculated and then compared to the grain boundary energy and stored energy of the three tiles if they were to form a strain-free grain. Figure 3.3 shows the situation of forming an energetically favorable grain where Eq. (3.6) is satisfied. In the figure, the various colors separated by thick black lines represent three different grains separated by general grain boundaries. The numbers inside of each tile correspond to the amount of stored energy present in each tile. It is important to note that the tiles with zero strain energy simulate the nucleation of a strain free grain.
Figure 3.3: During simulated recrystallization, a random tile and two neighboring tiles are chosen and tested to see if it is energetically favorable to nucleate. Should the conditions be favorable to form a nucleus, a strain-free grain is formed and the stored energy is set to zero. (a) shows the initial microstructure and (b) shows the microstructure after a nucleus is formed. Each color represents a separate grain. The numbers within the tiles represent the stored energy.

In order to determine whether or not forming a nucleus could be energetically beneficial, a number of other processes take place. During the simulation, the type of boundary along which the nucleation takes place is recorded and allows insight into the effect of special boundary fraction on recrystallization and vice versa. Another feature included in the simulation was the ability to force a nucleus to form a $\Sigma 3$ boundary with one of its neighbors. This was done by back-calculating the orientation required to form a $\Sigma 3$ on the orientation matrix of a random neighbor, and then assigning the calculated Euler angles to the new grain. The frequency of formation of nuclei with forced $\Sigma 3$ boundaries can be controlled by an input at the beginning of simulation (i.e., inputting a value of 15 would force 15% of the nuclei to have orientations that form $\Sigma 3$ boundaries). While the ability to force the formation of a $\Sigma 3$ boundary was added, it was not utilized in this work except to examine the effect it would have on the special boundary fraction (discussed further in Section 4.4).
The portion of this thesis that deals with the study of DRX kinetics requires information that tracks the onset and progression of recrystallization. While subsequent recrystallization cycles may differ between samples with high special boundary fractions and those with low fractions, it is the initial recrystallization cycle that is of interest. After the initial cycle, the special boundary fraction of both the high-fraction and low-fraction samples is similar. This means that the effect of special boundaries on DRX kinetics will be most evident during the first cycle. The equation to calculate the percent of grains that have been recrystallized is:

\[
\%_{\text{recrystallized}} = \frac{n_{\text{rx}}}{n}
\]

where \(n_{\text{rx}}\) is the number of tiles in recrystallized grains and \(n\) is the total number of tiles in the sample.

### 3.4 Grain Growth Algorithms

The mathematics behind the simulated grain growth mechanics is simpler than the recrystallization algorithm. While recrystallization was very computationally intensive, requiring information from 12 separate tiles and multiple matrix operations to determine whether or not it is favorable to nucleate at a test site, the implementation of grain growth into the simulation involves only two tiles. Similar to recrystallization, grain growth also follows an energy-based decision process. Once a random test site is selected (for grain growth, a “test site” is comprised of two tiles), the simulation calculates the energy of the tiles in their existing orientations and then assigns the orientation of the initially selected tile to its neighbor and recalculates the energy. If the reassigned orientations result in a lower energy than the original ones, the simulation then must decide whether or not the favored orientations are kept or not. Kinetics then determines how often reassigned orientations are retained or returned to their original orientations.
Unlike the kinetics of recrystallization, grain growth kinetics do not depend solely on the formation energy. Should a test site be found where the change in energy between the initial situation and a situation where grain growth occurs, only a certain percentage of favorable grain growth operations are retained. Whether a favorable grain orientation reassignment is retained or not depends on the following equation:

\[
P(\Delta E) = \begin{cases} 
  \text{not retained} & \text{if } \Delta E > 0 \\
  \text{retained} & \text{if } \Delta E \leq 1 \text{ and } \frac{\kappa}{\epsilon^2} \geq 1 
\end{cases} 
\]  

(3.8)

where \( \epsilon \) is an integer selected at the start of the simulation as part of the test parameters and \( \kappa \) is a random integer chosen between zero and \( \epsilon \). With regards to the physical interpretation of \( \epsilon \): larger values means slower grain growth.

The energy calculations of grain growth do not rely solely on the values of boundary energy, but also on the value of stored energy present in the grain. For example, nucleated grains have their stored energy reset to zero. A grain with little to no strain energy will be much more likely to grow than a heavily strained grain. However, as a grain grows, it will be affected by the strain of the neighboring grains. Should a grain growth operation be retained, the chosen tile next to the sample site is assigned the same orientation as the sample tile. Strain energy in the adjacent tile is averaged between its original value and the value of the sample tile. Figure 3.4 shows how the grain growth algorithm averages the stored energy between the two grains present in random location chosen during the Monte Carlo step.

Yet another factor of determining grain growth is the curvature of the grain boundary. All aspects being equal between two neighboring grains, a grain with a larger radius of curvature will be more likely to grow at the expense of a grain with a small radius of curvature. In order to
simplify calculations, and rather than explicitly calculating the radius of curvature of two grains at a sample site, the number of tiles present in each grain were compared and the grain with more tiles was assumed to have a larger radius. The energy associated with curvature, $E_c$, is described as:

$$E_c = \frac{n_A - n_B}{\max\{n_A, n_B\}}$$  \hspace{1cm} (3.9)$$

where $n_A$ is the number of tiles in the grain associated with the initially selected tile and $n_B$ is the number of tiles in the grain associated with the neighboring tile. Should $n_A$ be larger, the chance of grain growth is increased due to the added energy associated with curvature. However, the value of $E_c$ would be negative if the value of $n_B$ was larger than $n_A$ and therefore would hinder grain growth at that particular site. The equation for curvature limits the value of $E_c$ to either ±1, but the actual effect can be further reduced depending on the type of boundary present. It is known that high-angle general boundaries are more mobile than low-angle and special boundaries [17]. In the simulation, this means that low-angle and special boundaries

Figure 3.4: Schematic of (a) Two neighboring grains (denoted by red and blue colors) with differing stored energy values. (b) The left grain grows by a single tile (hexagon) and the stored energy of that tile is an average of the two tiles chosen as a possible grain growth site.
would be more resistant to the effects of curvature. Table 3.2 shows the reduction of the effect of curvature based on boundary type. Overall, a balance had to be achieved between the effect of grains that have already grown substantially against the effect of a newly nucleated grain that has a substantially smaller radius of curvature but is strain-free in order to ensure that newly nucleated grains “survived” in the simulation.

Table 3.2: List of grain curvature coefficients. Higher Σ boundaries are more mobile and therefore the effect of curvature would have a greater effect.

<table>
<thead>
<tr>
<th>Σ</th>
<th>$E_c$ Coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>Σ1</td>
<td>0.1</td>
</tr>
<tr>
<td>Σ3</td>
<td>0.1</td>
</tr>
<tr>
<td>Σ9</td>
<td>0.2</td>
</tr>
<tr>
<td>Σ27</td>
<td>0.3</td>
</tr>
<tr>
<td>High-angle</td>
<td>0.5</td>
</tr>
</tbody>
</table>
4 RESULTS AND DISCUSSION

4.1 Initial Microstructure

Two initial microstructures were obtained from EBSD scans of separate samples of 316L stainless steel and are shown in Figure 4.1. One of the samples underwent a single grain boundary engineering process while the other sample underwent multiple grain boundary engineering (GBE) processes. During GBE, the special boundary fraction significantly increases, as shown in Table 4.1. Each GBE process a material undergoes further increases the fraction of special boundaries. The “low-fraction” and “high-fraction” samples have been labeled according to their respective initial special boundary fraction. The initial average grain size for each sample is relevant as significantly different average grain sizes can affect the kinetics of DRX. The samples chosen for this research deviate by only approximately 11 tiles per grain (the low-fraction sample is approximately 13% smaller than the high-fraction). It has been determined that the average grain size between the samples is similar enough to reduce the effect of grain size, allowing the effect of special boundaries to be more pronounced.

Table 4.1: Special boundary information for starting microstructure.

<table>
<thead>
<tr>
<th></th>
<th>Special Boundary Fraction (% by length)</th>
<th>Σ3 Fraction (% by length)</th>
<th>Initial Avg. Grain Size (# of tiles/grain)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low-Fraction</td>
<td>69.8</td>
<td>56.5</td>
<td>76.06</td>
</tr>
<tr>
<td>High-Fraction</td>
<td>82.1</td>
<td>68.3</td>
<td>87.39</td>
</tr>
</tbody>
</table>
Figure 4.1: Experimentally obtained EBSD scan of 316L Stainless Steel for (a) a sample that has undergone a single GBE cycle and (b) a sample that has undergone three GBE cycles. Solid colors represent grain orientation while thin lines represent grain boundaries. Black grain boundaries are general boundaries while red are $\Sigma 3$ boundaries.

4.2 Simulating Experimental Trends in DRX

The unique characteristic of DRX is the multi-peak behavior of the stress-strain plots. However, with increasing strain rate, the stress-strain plots transition to single-peak and then, with a substantially higher strain rate, plots with no peak. Figure 4.2 shows the effect of altering the nucleation rate of the low-fraction sample for a fixed strain rate ($\dot{H} = 0.0002$) while Figure 4.3 shows that maintaining a constant nucleation rate of 2 nucleations per MCS causes the simulation to demonstrate behavior similar to experimentation (decreasing strain rate encourages multi-peak behavior and shifts decreasing peak values to the left). By varying the nucleation rate, the cyclic behavior can be adjusted to be more pronounced (with higher nucleation rates) or less pronounced (with lower nucleation rates) as seen in Figure 4.2. Higher nucleation rates allow more rapid removal of stored energy by means of forming strain-free grains. By reducing the nucleation rate parameter, nuclei are prevented from forming immediately once it is energetically favorable to nucleate. Delaying nucleation in turn delays the onset of DRX.
Figure 4.2: Simulations of the low-fraction sample showing that increasing the nucleation rate decreases the cyclic behavior for constant temperature and strain rate. Also, higher nucleation rates increase the peak stored energy value and delay the number of Monte Carlo steps where the peak value occurs. The simulation was anisotropic with a strain rate of 0.0002.
Figure 4.3: Simulations of the low-fraction sample showing that decreasing the strain rate also decreases the cyclic behavior for constant temperature and nucleation rate. This also decreases the peak stored energy value, and shortens time until the peak value occurs (i.e., shifts the peak to the left).
During simulation, the number of original grains present at every MCS were compared to the initial number of original grains. This provides a method of tracking the kinetics of recrystallization and allows microstructures showing various stages of recrystallization to be shown with the average stored energy as a function of time. As shown in Figure 4.4, the majority of the first recrystallization cycle occurs during the first peak. This matches expected behavior where portions of a stress-strain curve with a positive slope correspond to grain growth dominated behavior while negative sloped portions are where recrystallization occur.

Figure 4.5 shows evidence that the trends observed in experiments are also found in the simulation. The characteristic DRX behavior of stress-strain curves transitioning from single-peak to multi-peak behavior with decreasing strain rate and/or increasing temperature is replicated reasonably well. Due to the ability to model the general behavior of DRX, the details behind the mechanisms of DRX and the related changes to microstructure can be observed, compared to experimental results, identified, and then characterized in a way to allow the microstructural changes to be predicted.

The data from each simulation allowed the extraction of the peak average stored energy and allowed analysis of the magnitude of the peak. Figure 4.6 shows the maximum peak and the strain rate at which it occurred. The highest peak values correspond to the largest strain rates. This is most likely due to the fact that higher strain rates increase the stored energy faster than can be initially removed by grain growth and recrystallization. The higher strain rate also increases the difference between the high and low-temperature peaks.

4.3 Temperature Effects

It has been shown experimentally that temperature affects DRX. Figure 4.5 shows the qualitative effect of temperature at various strain rates. At higher strain rates, the effect of temperature is significantly greater than that at lower strain rates. For lower strain rates, the system is able
Figure 4.4: Average stored energy for low-fraction sample with accompanying microstructure maps. The percentage next to the microstructure maps refers to the amount of new grains when compared to the original grains. For example, 25% means that 25% of the original grains have been removed due to grain growth and recrystallization. The various colored grains correspond to various grain orientations while the lines between the grains correspond to grain boundary types. Black lines are general boundaries while red lines are special boundaries.
Figure 4.5: Simulations of the expected behavior for (a) and (b) of decreasing average stored energy with increasing temperature holds true for the simulated results except for exceptionally low strain rates; this trend stands for both the high-fraction and low-fraction samples.
Figure 4.6: Simulations of the maximum stored energy plotted for each materials at varying strain rates and temperatures. The effect on the peak average stored energy due to temperature and nucleation rate are greater at higher strain rates. Note that lines are not trend lines.
to remove the strain energy efficiently with even the lowest grain growth and nucleation rates. However, at higher strain rates, the higher grain growth and nucleation rates that occur during the high temperature simulation are able to achieve a steady state average stored energy more quickly.

Figure 4.5 shows the effect of temperature for the low and high-fraction samples at various strain rates. In both samples, the low-temperature peaks are higher and shifted to the right. A shift of the peak to the right implies that the recrystallization portion of the simulation is delayed. This is due to the lower nucleation rates. At lower temperature, nucleation attempts occur less frequently and the stored energy in the simulation must reach a sufficient level such that every nucleation attempt results in a successful nucleation. At higher temperatures, the nucleation rate is higher and therefore a favorable nucleation location may be found earlier in the simulation.

### 4.4 Effect of Special Boundary Fraction

Including the effects of special boundaries in this work required the use of anisotropic grain boundary energy. The most obvious method with which to observe the effect of special boundaries is to compare an isotropic simulation to an anisotropic run using the exact same parameters for temperature, strain rate, and forced $\Sigma 3$ formation. Figure 4.7 shows the effect of initial special boundary fraction compared to isotropic simulations on the rate of recrystallization for both samples. The figure shows that the onset of recrystallization is delayed for both samples when grain boundary energy is taken into account (anisotropic case). However, the delay is extended further for the high-fraction sample, where the difference in the total grain boundary energy in the sample between the isotropic and anisotropic simulations is greatest. This plot shows that the effect of grain boundary energy can alter the kinetics of DRX by delaying the onset of recrystallization. The reason for this is that the presence of special boundaries in the microstructure significantly lowers the number of favorable nucleation sites. As stated earlier, the recrystallization algorithm
requires that the energy of the nucleus being formed be less than the energy previously present at the nucleation site. The presence of even a single special boundary reduces the desirability of a nucleation site a significant amount. In order to nucleate at a site with a special boundary, the stored energy removed by the nucleation of a strain-free grain must offset the energy gained by forming (most likely) a nucleus enclosed in general boundaries.

![Figure 4.7](image)

**Figure 4.7:** Comparing rates of recrystallization for isotropic and anisotropic simulations. Both the low and high-fraction samples showed that recrystallization was delayed for anisotropic simulations when compared to isotropic runs. The delay in recrystallization is more pronounced for the high-fraction sample.

Figure 4.8 shows plots of both the low and high-fraction samples at identical temperatures and strain rates. The high-fraction samples consistently have lower maximum average stored energy values than the low-fraction sample around the peak average stored energy values. However, after the peak values, the steady state values between the two samples were similar for all strain rates.
While it may seem to be a result that runs counter to what is expected (since special boundary fraction was expected to result in different behavior), the difference in special boundary fraction is removed after the first recrystallization cycle. Once the special boundary fractions become similar in the two samples, it stands to reason that their average stored energy values between the two samples would be similar. As the initial microstructure is replaced by grains of random orientation, the special boundary fraction decreases in all situations to a similar percentage.

**Figure 4.8:** Plot of low and high-fraction samples at the same temperature and strain rate. Note that the energy peaks for the high-fraction samples are lower and shifted to the right when compared to energy peaks for the low-fraction sample. Physically, this would correspond to an earlier onset of DRX.

The variation in peak energy values in Figure 4.8 is quantified more directly in Figure 4.9. The positive slopes observed in both plots indicate that the trend associated with initial grain boundary fraction and maximum average stored energy may be similar to the relationship that has been observed between initial grain size and the maximum stresses observed [5]. Previous work found that smaller initial grain sizes in DRX experiments caused stress-strain curves to
have lower stress values and the peak stress value were shifted to the right. It was concluded that this was due to smaller grain sizes providing more nucleation sites [5]. Conversely, the delay in the maximum peak value for larger grain sizes corresponded to a delay in the onset of DRX and was hypothesized to occur due to the lower number of nucleation sites. From these observations, it appears that the initial special boundary fraction alters the effective initial grain size: higher initial special boundary fractions effectively increases the initial grain size.

![Graphs](image)

**Figure 4.9:** Comparing special boundary fraction to (a) the maximum average stored energy as well as (b) the time required to reach the maximum average stored energy. The data shows that there may be a similar correlation between the effect of special boundaries and the effect of initial grain size: higher special boundary fractions have the potential to have a similar effect as larger initial grain sizes.

Simulations that used the parameter controlling whether or not a nuclei was forced to form a $\Sigma 3$ boundary were also run. Figure 4.10 shows that for both samples, the steady state special boundary fraction is similar despite the varying initial fraction. The increased fraction of formation slowed the decline of the special boundary fraction and slightly increased the steady state fraction. These results are what is expected due simply to geometry. After the first recrystallization cycle, there is an abundance of triple junctions on which to nucleate. Assuming every
nucleus forms a \( \Sigma 3 \) boundary with a neighboring grain, and assuming all boundaries are of equal length, the maximum possible special boundary fraction would be 30%. However, since the special boundary fraction is calculated by length, and not all boundaries are of equal length, a steady state fraction of special boundaries around 22% seems reasonable after recrystallization.

The reason for this direct relationship between initial special boundary fraction and the onset of recrystallization is due to the relationship between the low energy of special boundaries and the effect they have on decreasing the desirability of forming nuclei on them. Since nucleation occurs along grain boundaries, lower energy at these sites mean that it is more efficient for the system to continue to attempt grain growth rather than nucleation until the stored energy reaches a point where forming boundaries around a strain-free grain is more favorable.

The reason for the change in the special boundary fraction can be attributed to the introduction of energetically preferable boundaries. By forcing low-energy boundaries to form during recrystallization, the number of preferred nucleation sites in the system is decreased. In order for a nuclei to form on a non-preferred site, the strain energy within a grain must increase to the point at which the grain boundary energy becomes irrelevant. This means that the simulation must progress longer to add the necessary strain and therefore the rate at which the special boundary fraction decreases is diminished. The steady state value for the special boundary fraction is also increased due to the presence of energetically favorable boundaries.

### 4.5 Nucleation Location and Available Nucleation Sites

Simply tracking the location of each nucleus formed during DRX is not enough to draw relevant conclusions about preferred nucleation location. Another factor that must be taken into account is the availability of each type of nucleation location. Each sample undergoes the first DRX cycle at approximately 10,000 MCS and therefore the data in the following figures show
Figure 4.10: Comparison of the effect of forcing a percentage of new nuclei to form $\Sigma 3$ boundaries with a random neighbor in both the high- and low-fraction samples. Simulations were conducted at the same temperature and strain rate for both samples. Higher percentages of forced $\Sigma 3$ boundaries slow the decline of the overall special boundary fraction and increase the steady state fraction.
information for the first cycle of each sample before the variations in special boundary fraction between the two samples are removed by complete recrystallization.

Figures 4.11 to 4.14 compare the available nucleation sites with the location where nucleation actually occurs. If the possibility of nucleating at a triple junction was random, then the fraction of nucleations at triple junctions would be directly correlated to the number of triple junctions present. The figures show that triple junctions, particularly J0 triple junctions, are preferable nucleation sites. The shaded portions of Figures 4.11 to 4.14 denote a portion of the simulation that is dominated by grain growth. During this period, very few, if any, nuclei are formed. The graphs on the right-hand side compare the percentage of available sites (light colored bars) with the percentage of nuclei that are formed at each site (darker colored bars). In every simulation, the number of nucleations at a triple junction is higher than the fraction of available triple junction sites. Also, the percentage of nuclei that form specifically at J0 triple junctions is higher than the initial percentage of available J0 sites.
**Figure 4.11:** Comparison of available nucleation sites to the actual location at which nucleation occurs for the low-fraction sample. The shaded area on the left plot denotes the portion of the simulation dominated by grain growth. Solid bars on right graph denote the fraction of nuclei that formed for each boundary type. Lighter bars denote initial fraction of available nucleation sites of each type at 4,000 MCS.
**Figure 4.12:** Comparison of available triple junction sites to the actual location at which nucleation occurs for the low-fraction sample. The shaded area on the left plot denotes the portion of the simulation dominated by grain growth. Solid bars on right graph denote the fraction of nuclei that formed for each boundary type. Lighter bars denote initial fraction of available nucleation sites of each type at 4,000 MCS. Only the peak percentage of available J0 sites fails to surpass the corresponding actual nucleation fraction.
**Figure 4.13:** Comparison of available nucleation sites to the actual location at which nucleation occurs for the high-fraction sample. The shaded area on the left plot denotes the portion of the simulation dominated by grain growth. Solid bars on right graph denote the fraction of nuclei that formed for each boundary type. Lighter bars denote initial fraction of available nucleation sites of each type at 4,000 MCS. While the percentage of available triple junction sites never reaches 15%, the percentage of nuclei that formed at a triple junction was closer to 25%. 
For an energetically driven system (where a system evolves toward lower total energy), it stands to reason that the most effective method to eliminate energy would be to eliminate that which contributes the most to the energy of the system as often as possible. In the case of microstructure, the highest energy is at J0 triple junctions due to the presence of three general boundaries. This means that even though the fraction of available nucleation sites that are triple junctions is low, there is a higher than random possibility of nucleating at a J0 triple junction. In short, the simulation shows that for both the high and low-fraction samples, nucleation is preferred at triple junctions and, more specifically, J0 triple junctions due to the high energy
that can be found at these sites. Nucleating at these sites is more energetically efficient than nucleating at a site with lower energy boundaries. Conversely, in both samples, the fraction of nucleations on J3-type triple junctions is significantly lower than the available fraction of J3-type sites. In both samples, the highest fraction of actual nucleation occurs on J0 and J1 while the lowest occurs on J2 and J3 triple junctions. This is expected due to the energies at each site.
5 CONCLUSIONS

5.1 Implications

In conclusion, the simulation developed for this work is able to replicate several important trends observed in experimental DRX research. Previous work showed the importance of temperature, strain rate, and observation of nucleation occurring primarily on grain boundaries [8, 11]. This work was able to simulate the effect of temperature and strain rate and successfully show that increasing temperature and decreasing strain rate lower the average stored energy and plotted curves transition from single-peak to multi-peak. This work also showed that nucleation occurred at grain boundaries in necklace structures.

A step towards bridging the gap between experimental and simulational results was achieved by accepting experimental EBSD scans as initial microstructure. From these scans, it was possible to calculate grain boundary energy based on grain misorientation to allow for simulation of anisotropic boundary energy. Over the course of the simulation, it was possible to track nucleation location and separate into triple junction vs. non-triple junction locations and differentiate between four types of triple junctions (J0, J1, J2, and J3).

One of the important results obtained in this work is that the presence of special boundaries delays the onset of recrystallization due to the low energy of special boundaries being unfavorable for nucleation. Noting a similar delay in recrystallization in experimental work examining the effect of initial grain size allowed a comparison of initial special boundary fraction and initial grain size. It may be possible to derive an “effective grain size” by including both grain size and special boundary fraction. Also, the simulation was able to show that triple junctions are prefer-
ential nucleation locations (as shown experimentally [8]). Specifically, nucleation is favored at lower J-value triple junctions (i.e., J0, J1).

5.2 Future Work

To continue improving this simulation, it is recommended that a method be developed to correlate “Average Stored Energy” to stress and “Monte Carlo Steps” to strain. Since this work ignored material composition, it would be advantageous to implement material specific parameters that accurately model DRX for various other materials. One suggested method for accomplishing this would be to include a coefficient that could be applied to the grain growth/strain rate/grain boundary energy parameters that would effectively scale the parameters to alter the simulation to match experimental results. Previous experimental work has also shown the effects of impurities [11] on DRX. This could be modeled by allowing different grains to behave differently than the bulk material. It is believed that the current work could be modified to accomplish most of the work listed here with moderate effort.
REFERENCES


