IMPROVING THE FUNCTION FOR GRAIN BOUNDARY ENERGY INTERPOLATION IN URANIUM DIOXIDE

by

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DEPARTMENT APPROVAL

of a senior thesis submitted by

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This thesis has been reviewed by the research committee, senior thesis coordinator, and department chair and has been found to be satisfactory.

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ABSTRACT

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Efforts have been made to find an interpolary function for the grain boundary (GB) energies of uranium dioxide, based on work done by Bulatov *et al.*[Acta Mater. 65, 161 (2014)]. A MATLAB® script was developed based on Harbison[B.S. Thesis, Brigham Young University - Idaho (2015)] and Bulatov *et al.* to perform this work. Molecular dynamics data was collected using the LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulation) program developed at Sandia National Laboratory. Results for the ⟨100⟩, ⟨110⟩, and ⟨111⟩ symmetric tilt and twist GBs have been collected. The new data sets were calculated with an 800 K anneal which allowed the atoms to relax to a lower energy state. An improved fit is found for the ⟨100⟩ and ⟨110⟩ symmetric tilt sets and the ⟨110⟩ twist set, whereas the ⟨100⟩ twist and ⟨111⟩ symmetric tilt and twist sets show unexpected trends. Further research needs to be done for the ⟨100⟩ and ⟨111⟩ sets to determine why the fitting procedure does not accurately reflect the expected results. Additional research should also be done to determine if outlying data points necessitate fitting additional cusps.

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Chapter 1

Introduction

Uranium dioxide (UO_2) is the primary choice for nuclear fuel in today's reactors.[1] Understanding the properties of UO_2 requires an analysis of the basic crystal structure of the material. UO_2 is a ceramic (a type of polycrystalline material), meaning that a series of crystal lattices join together in various ways (called twist, tilt, or mixed boundaries) to create it. This material has a fluorite crystal structure, where the uranium atoms form a face-centered cubic (fcc) lattice, and the oxygen atoms form a simple cubic lattice within the fcc frame (see Figure 1.1).

The various properties of the fuel need to be well understood to make running the reactor as safe and effective as possible. Some of these properties include thermal conductivity (how well heat flows through the material), fission gas release (how some of the fission products move throughout the material as gases), and mechanical stability (i.e. how the material bends or cracks under pressure or heat). Taking thermal conductivity as an example, knowledge of this material property allows the most effective use of coolant to keep the reactor within operating temperatures, maximizing both efficiency and safety. Knowledge of other material properties allows for similar gains in efficiency, safety, or both.

Interest in understanding UO_2 while in-reactor has lead to efforts to more deeply understand the properties of the material. Currently, Idaho National Laboratory (INL) faces the

challenge of not having a complete model of grain boundary energy anisotropy. The current model assumes an isotropic energy, and this leads to an inability to model the material parameters correctly while in-reactor. This in turn makes efforts in nuclear energy less efficient and/or safe than it otherwise could be. The goal at INL is to accurately model nuclear fuel while in-reactor, allowing accurate predictions regarding how the material properties will change.

This work adds to the safety and efficiency of using nuclear energy by providing the necessary information to accurately calculate the material properties of UO_2 in-reactor. Specifically, this work improves the fitting parameters for grain boundary (GB) energy interpolation for UO_2 by using molecular dynamics (MD) results calculated by Zhang[2] and Hansen[3] with an anneal of 800 K. Furthermore, this work begins preliminary efforts towards using more accurate functions to describe GB energy behavior. Previous data did use annealed crystal structures,[4] which prevented the atoms from finding their ideal energetic minimum. The 800 K anneal allows the atoms to relax to a value closer to their global minimum, as shown in Chapter 3. A database will store these simulated energies, and a MATLAB® script will use the database to fit the function parameters. Idaho National Laboratory (INL) will incorpoate the updated parameters into its mesoscale phase field modeling platform MARMOT for use in modeling nuclear fuels. As these parameters are implemented in the modeling software, various tests of the UO_2 fuel can determine how the material properties change while in-reactor.

1.1 Background

Polycrystalline materials (ceramics, metals, and polymers) are composed of tiny crystals called *grains*. The orientation of each grain is generally independent of the orientation in the grains surrounding it. Therefore, there is a possibility (depending on how the crystal formed[5]) that crystal structures will not line up at the interfaces where these two grains meet.

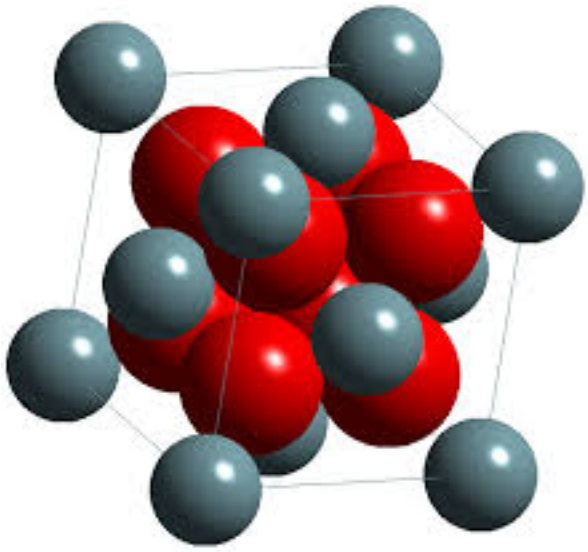


Figure 1.1 An image representing the fluorite crystal structure. For UO_2, the smaller spheres indicate the uranium atoms, and the larger spheres indicate the oxygen atoms. Image courtesy of the University of Cambridge under the Creative Commons license.

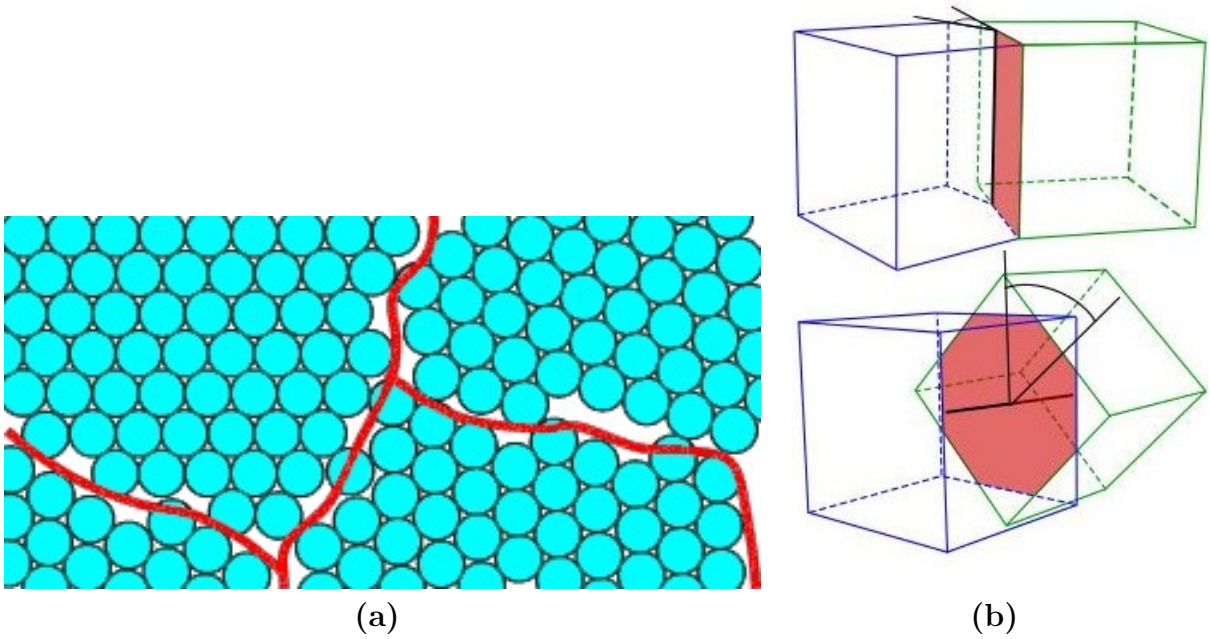
This "atomic mismatch"[5] leads to broken or stretched atomic bonds where atoms will not line up relative to a perfect crystal structure. These defects are called grain boundaries (GBs), and an illustration of a GB is shown in Figure 1.2a. The most popular way to parameterize a GB uses the five degree-of-freedom (DoF) model.[4,6–10] This model only uses the macroscopic DoFs (the observable DoFs corresponding to the misorientation and inclination), ignoring the three translational DoFs (the ability of the grain to move or slide anywhere in space) possessed by each grain. Three of the five DoFs specify the misorientation (or misaligment) of the grains with respect to each other. The other two DoFs specify the orientation of the grain boundary plane (called the inclination). The rotation axis and angle define the misorientation DoFs, and the GB normal defines the inclination DoFs.[7]

Three specific types of GBs occur in polycrystalline materials: twist, tilt, and mixed GBs.[7,10] These GBs desribe the misorientation of two grains with respect to each other. Twist boundaries have the axis of rotation between the two grains and the GB normal parallel to each other. Tilt boundaries can be either symmetric and asymmetric. A tilt

boundary occurs when the axis of rotation between the two grains is perpendicular to the GB normal. Symmetric tilt boundaries describe a GB whose boundary plane is a mirror plane: the atoms on one side of the boundary plane mirrors the other side. This makes the angles between the boundary plane and the orientation axes of the two grains equal. Asymmetric tilt boundaries have unequal angles. Figure 1.2b shows a representation of tilt boundaries (top) and twist boundaries (bottom). A mixed GB combines twist and tilt boundary characteristics.

Understanding GBs is important because of the effects they have on material properties.[6,8,9] The crystal structure has extra energy because of the atomic mismatch at the boundaries. This extra energy, called GB energy, gives rise to GB motion. Knowing and predicting how the GBs will move allows for more accurate calculations of a material's properties. Thus, GB energy needs to be understood to accurately model the evolution of material properties.

Two methods of modeling GB energy are the isotropic and anisotropic models. The most common method (and easier method) is the isotropic model. This model ignores the impact of inclination on the GB energy, and assumes equal inclinations for a given misorientation, reducing the five-dimensional (5D) parameter space to a three-dimensional (3D) parameter space. The reasons for assuming this model historically were based on the assumption that the inclination had little or no impact on the GB energy, or (later) that it was too difficult to create a full five DoF model.[8] Alternatively, the anisotropic approach seeks to quantify the effect that misorientation *and* inclination have on the GB energy. Currently, researchers acknowledge the need for a full five DoF model for GB energy, but assert the difficulty inherent in developing such a model.[7,8,10] Despite these difficulties, GB energy functions for certain materials, namely fcc metals copper, gold, aluminum, and nickel, have proven successful.[9]



(a) (b)

Figure 1.2 A representation of GBs, where (a) shows an example of a grain boundary and (b) shows an example of GB types. In (a) circles represent individual atoms of the grains, and the line represents the grain boundary. Atomic mismatch between the differently oriented grains causes an excess of energy within the material, which has an effect on the material's properties. Image courtesy of the University of Cambridge under the Creative Commons license. In (b) the axis of rotation for the tilt GB (top) is perpendicular to the GB normal, and for the twist GB (bottom) is parallel to the GB normal. Image courtesy of Wikipedia under the Creative Commons license.

Chapter 2

Methods

Sufficient data is a requirement for any fitting procedure, but unfortunately there is a lack of data on uranium dioxide (UO_2) grain boundary (GB) energies in the literature. As a work-around, this work used molecular dynamics (MD) simulations[2,3] as fitting data to calculate the GB energies of various lattices based on the coincident site lattice (CSL) model. This model builds off of the idea that the GB energy has lower values when more lattice sites coincide. A number defined as the Σ-number describes the number of coincident sites per total number of lattice sites in a given unit cell of a crystal.[7,10] This work developed a MATLAB® script using Bulatov *et al.*'s methods[9] and building off of Harbison's script[4] to fit parameters to the gathered data. A reduced chi-square statistic was calculated to determine the effectiveness of the fit.

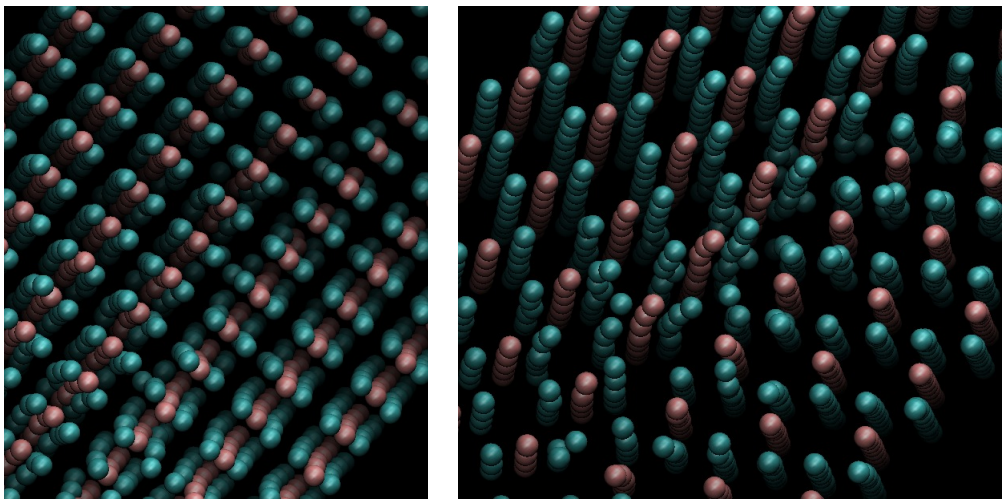
2.1 Molecular Dynamics

Simulation results from the Large-scale Atomic/Molecular Massively Parallel Simulation (LAMMPS) software (developed at Sandia National Laboratory[11]) were gathered for a number of twist, tilt, and mixed GBs. These calculations were performed by simulating two crystals of UO_2 and placing them together in various orientations. A GB is introduced at the interface, creating GB energy. The energy of the system is calculated from the inter-

atomic forces inside the crystal. Comparing that energy to the energy of a single grain (of the same size as the combined two grains) of UO_2 determines the energy at the GB.[4] The GB energy is calculated as:[12]

$$E_{\mathrm{GB}} = \frac{|E_{\text{single grain}} - E_{\text{two grains}}|}{2A_{\mathrm{GB}}}. \tag{2.1}$$

An example of how the atoms align is shown in Figure 2.1. Harbison's original calculations[4] were done using no anneal ($T_{\max} \approx 0$ K), only allowing the atoms to relax to their local minima. This work used an anneal of 800 K, allowing the atoms to relax to a better estimate of their global minimum value as shown in Chapter 3. This work used the same misorientation angles for the GB energy calculations that Harbison used. The fitting procedure uses these energies to produce parameters describing the five-dimensional GB space.



(a) **(b)**

Figure 2.1 These figures demonstrate example crystal structures of UO_2 after an annealing process. The better the atoms line up, the lower the energy. (a) shows an example of a mostly aligned GB, indicative of a lower energy. (b) shows an example of a misaligned GB, indicative of a higher energy. These two images are from a $\langle 111 \rangle$ twist image. Different viewpoints show different amounts of alignment. The LAMMPS simulation package takes care of all the calculations to determine the energy at these GBs. Images courtesy of Dr. Evan Hansen, used with permission.

2.2 Bulatov *et al.*'s Methods

This work implemented Bulatov *et al.*'s hierarchical interpolation method to find the energy of an arbitrary GB in the five-space.[9] They chose three three-dimensional (3D) axes with at least two-fold symmetry (called high-symmetry axes) to use as scaffolding to build the entire five-dimensional (5D) function. The axes chosen for both Bulatov *et al.* and this work were the ⟨100⟩, ⟨110⟩, and the ⟨111⟩ sets for their four-, two-, and three-fold rotational symmetries respectively.* Each 3D subset builds from interpolation of its own one- and two-dimensional subsets. The symmetric tilt and twist GBs for each set were fitted first because of their simplicity. The rotation angle fully defines the energies for these subsets, making them one-dimensional (in Figure 2.2a, the darker bands in the smaller circles). From the symmetric tilt subset, the asymmetric, or general, tilt subset was interpolated. A second rotation angle defining the rotation of the second grain makes this subset two-dimensional (the lighter, wider band of color around the symmetric subset). A combination of the general tilt (two dimensions) and the twist subsets (one dimension) interpolates the 3D subset for each high-symmetry axis (the three smaller circles). These three 3D subsets were then used to interpolate the GB 5D space. Figure 2.2b shows the simplified GB space using the Rodrigues fundamental zone representation.

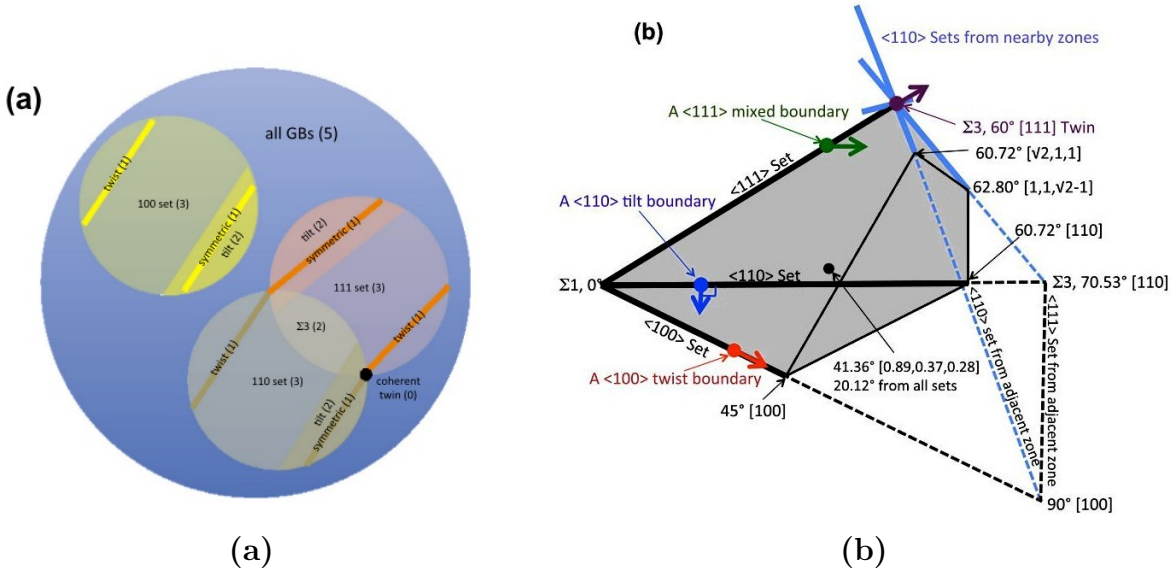
Bulatov *et al.* and this work used the Read-Shockley-Wolf (RSW) functions,[14] which take the form:

$$E_{min} + (E_{max} - E_{min}) \sin\left(\frac{\pi}{2}\frac{\theta - \theta_{min}}{\theta_{max} - \theta_{min}}\right)\left(1 - a\log\left(\sin\left(\frac{\pi}{2}\frac{\theta - \theta_{min}}{\theta_{max} - \theta_{min}}\right)\right)\right), \quad (2.2)$$

where θ is the misorientation angle, θ_{min} is the minimum angle on the domain, θ_{max} is the maximum angle on the domain, a is a shaping parameter, and E_{min} and E_{max} represent the energy at θ_{min} and θ_{max} respectively. Each RSW function covers a "low-angle" subset

*For cubic crystals, rotations of 90°, 180°, or 120° about any ⟨100⟩, ⟨110⟩, or ⟨111⟩ axis respectively is a symmetry operation.[13] Thus, the ⟨100⟩ set is four-fold symmetric (360°/90°= 4), the ⟨110⟩ set is two-fold symmetric (360°/180°= 2), and the ⟨111⟩ set is three-fold symmetric (360°/120°= 3).

(around 15°, with higher angles being less accurate)[10,14] of the domain in the 1D GB space. An example of a simple RSW function is shown in Figure 2.3. Multiple RSW functions are stitched together to form the 1D subsets.



(a) (b)

Figure 2.2 Figure 2 from Bulatov *et al.*[9] (a) demonstrates the theoretical relationship between the high-symmetry subsets of the 5D GB space. Each multi-dimensional subset is interpolated from smaller-dimensional subsets. (b) shows the Rodrigues space representation of the fundamental zone of all GBs as built from three high-symmetry axes (⟨100⟩, ⟨110⟩, and ⟨111⟩). The unit vectors along the axis identify the boundary plane inclination in the frame of grain one. A parallel vector thus represents a twist boundary, a perpendicular vector represents a tilt boundary, and neither parallel nor perpendicular vectors represent a mixed boundary. The full misorientation space has 1152 symmetrically equivalent copies of the fundmental zone[9,15] which allows the infinite nature of Rodrigues space to be accounted for.

2.3 Code Analysis

Harbison[4] and Bulatov *et al.*[9] developed MATLAB® scripts for their work. This work analyzed these codes and used the ideas from them to develop the code that generated the parameters listed in Appendix A.

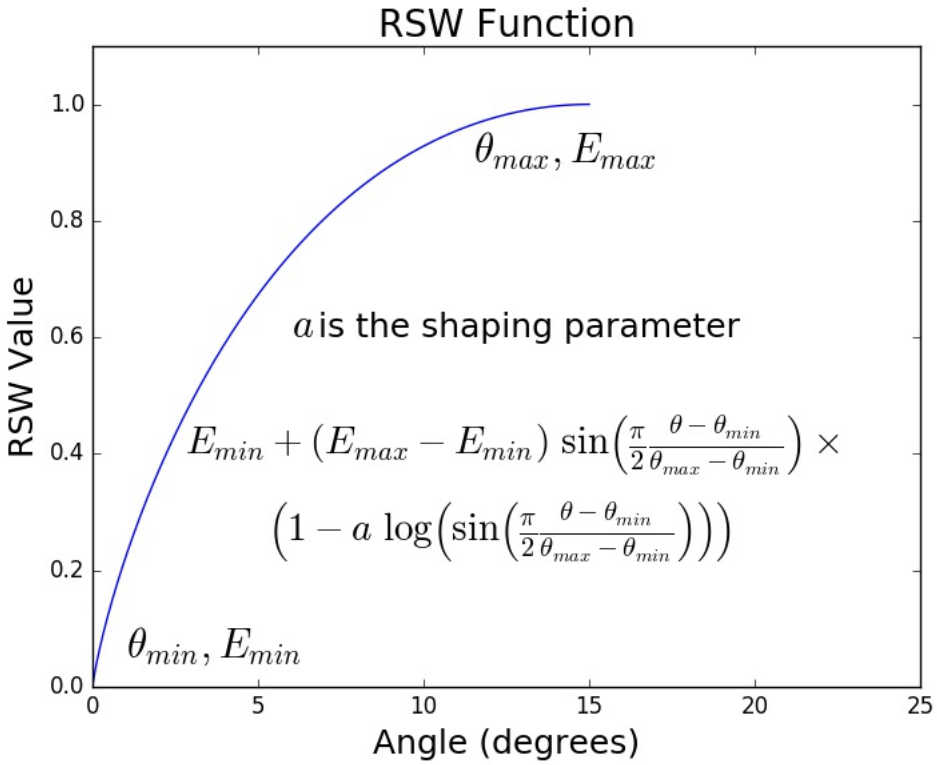


Figure 2.3 An example of an RSW function with $\theta_{min} = 0°$, $\theta_{max} = 15°$, and a (the shaping parameter) $= 0.5$ Combining these functions into a Piecewise set over a given domain gives the GB energy curves their distinct, cusp-like behavior. The RSW functions are scaled using E_{min} and E_{max}. In this example, $E_{min} = 0$ and $E_{max} = 1$. Note that E_{min} and E_{max} do not represent the lowest and highest energies in the domain, but rather represent the energy at θ_{min} and θ_{max} respectively.

2.3.1 The Fitting Code

This work performed an extensive analysis of Harbison's code to learn how it works and to implement the ideas therein. The basic outline for the fitting procedure follows. First, data is read in from a database containing energies associated with either a twist or tilt GB on one of the three high-symmetry axes. Test parameters, used as starting points for the fitted parameters, are also read in from a separate database. The parameters found from the 1D fits are used in fitting the higher-dimensional sets. Important angles specify where low energies are expected, such as the $\Sigma 5$ boundary for the $\langle 100 \rangle$ symmetric tilt subset. These angles are calculated based on the Σ-number from CSL theory. Because the Σ-number

designates how many lattice points are between each coincident site (and assuming that the space between each lattice site, the lattice constant, is known) the angle of the GB misorientation can be determined. Every energy in the parameter-vector is listed as a scaled value based on the e_{RGB} parameter to minimize the potential for error in calculations. The e_{RGB} parameter represents the energy of an arbitrary, random GB, and can be seen as an average of the material's GB energies. Thus, to make relevant comparisons, the energies are unscaled based on the units of energy desired (typically J/m^2). All of the parameters and the angle-energy pairs from the database are then passed into a grid-search fitting function. This work gave each subset a different initial step size to avoid a numerical error where the steps would take the angles currently being looked at outside of their domain. Without this, the grid-search procedure would not return the correct amount of values, preventing the code from running to completion.

Once the six one-dimensional subsets and the three two-dimensional subsets are fitted, the three-dimensional subsets are fitted using the twist and asymmetric tilt subsets to calculate the mixing parameters (defining the relationship between the twist and general tilt subsets within a high-symmetry axis - i.e. the relationship between the small dark bands representing the twist boundaries and the lighter, wider bands representing the tilt boundaries in Figure 2.2a). The final step calculates the weighting parameters, which defines the relationship between the three high-symmetry subsets. Equations defining the various relationships can be found in Bulatov *et al.*'s work.[9]

2.3.2 The Energy Calculation Code

Bulatov *et al.*'s open-source MATLAB® code,[9] `GB5DOF.m`, calculates the energy of an arbitrary GB in certain fcc metals. This work uses this script for calculating an arbitrary GB in UO_2, and proceeds as follows. First, metrics defining the "distance" between the GB and all three high-symmetry axes are calculated. These distances are calculated by looking at all symmetrically equivalent representations of a GB on a per-axis basis (for cubic crystals,

there are 24 equivalent representations[13]). Because there are three, six, and four unique axes for the ⟨100⟩, ⟨110⟩, and ⟨111⟩ axes respectively, a maximum of $6 \times 24 = 144$ distances are calculated. Any distances exceeding a predefined cutoff distance are discarded. After all distances have been calculated, only the unique representations are kept to avoid double-counting certain representations.[9] Energies are calculated for each unique distance in each subset. These energies are then weighted and summed to give the interpolated energy for the specified GB.

2.4 Reduced Chi-Square Statistic

A good way to test how well a function fits the data is to use a reduced chi-square goodness-of-fit statistic.[16] The orientation matrices (which Bulatov *et al.* calls the P and Q matrices for the first and second grains respectively) were needed as input parameters to Bulatov *et al.*'s function to calculate this statistic. These three by three matrices specify the orientation in a lab frame of the two grains individually. A good fit will have a reduced chi-square value close to one, while those values greater than one indicate an under fit, and those values less than one indicate an over fit.[16]

2.4.1 Developing the P and Q Matrices

This work created the P and Q matrices which was a non-trivial task. Because there has been so much work done with crystallography over the past few decades, many different methods have been developed to specify the orientation matrices of grains. A rotation matrix also needed to be calculated which rotates the axis of rotation to the [100] direction, as Bulatov *et al.*'s energy calculation code assumes. Three methods, following the method prescribed in MARMOT, using the Rodrigues rotation formula, and using the Bunge rotation matrix, were used in this work in the process of developing these matrices and are described below.

MARMOT Method

MARMOT, Idaho National Laboratory's (INL's) mesoscale phase-field modeling platform,[17] calculates the P and Q matrices for the grains using Euler angles as input parameters. The Euler angles are converted to the orientation matrices using the Bunge convention, i.e. the ZXZ or $ZX'Z''$ rotation, where the first rotation is about the z axis, the second rotation is around the new x axis, and the final rotation is about the new z axis. The formula for this conversion from Bunge Euler angles to the rotation matrix is found by multiplying the z, x, and z rotation matrices together in that order to get:

$$\begin{bmatrix} c_1\ c_3 - c_2\ s_1\ s_3 & -c_1\ s_3 - c_2\ c_3\ s_1 & s_1\ s_2 \\ c_3\ s_1 + c_1\ c_2\ s_3 & c_1\ c_2\ c_3 - s_1\ s_3 & -c_1\ s_2 \\ s_2\ s_3 & c_3\ s_2 & c_2 \end{bmatrix} \tag{2.3}$$

where c_{n} and s_{n} represent the cosine and sine of the respective angles (1 represents the first z rotation, 2 represents the x rotation, and 3 represents the second z rotation. These angles are usually referred to as[15] φ_1, Φ, φ_2).

The rotation matrix is calculated in MARMOT by using the GB normal and finding the rotation matrix required to rotate that vector to the [100] direction. In MARMOT, simulations are set up through input files. In the input files different sections (called blocks) specify material parameters, boundary conditions, initial conditions, and the physical models to use to solve the problem (among others). The initial condition used to calculate the rotation matrices in MARMOT for this set of problems was a horizontal or vertical line for tilt or twist boundaries respectively. Because of this set up, the GB normals were either along the [010] axis for the tilt boundaries, or $[\bar{1}00]$ for twist boundaries.

Rodrigues Rotation Formula

The Rodrigues rotation formula[18] (RRF) calculates the rotation matrices given an axis and an angle using the following formula:

$$\boldsymbol{R} = \boldsymbol{I} + \sin\theta\ \boldsymbol{K} + (1 - \cos\theta)\ \boldsymbol{K}^2, \tag{2.4}$$

where $\boldsymbol{I}$ is the 3x3 identity matrix, θ is the angle rotated through, and $\boldsymbol{K}$ is the skew-symmetric matrix formed by the axis of rotation ($\boldsymbol{a}$) by:

$$\begin{bmatrix} 0 & -a_z & a_y \\ a_z & 0 & -a_x \\ -a_y & a_x & 0 \end{bmatrix} \tag{2.5}$$

This work calculated the rotation matrices two different ways with this orientation matrix formulation. The first method simply used the MARMOT-generated rotation matrices. A second method calculated the rotation matrices using geometric arguments (see Figure 2.4). From the geometric arguments the normals are identified in Table 2.1. Appendix E shows the code used to generate the rotation matrices.

Bunge Rotation Matrix

MARMOT uses the Bunge rotation matrix (see Equation (2.3)) to create the orientation matrices. This work used various methods to calculate the Euler angles, of which three are briefly described here. The Euler angles (once calculated) were used in the first two methods to calculate the entirety of the rotation matrix.

First, this work tried to use scripts developed to calculate the various Euler angles for MARMOT. These scripts did not work because of the same assumptions made earlier about the orientation of the GB, namely, that all pure tilt GBs have a normal of 010, and that all pure twist GBs have a normal of $\bar{1}00$. The difference between MARMOT's boundary conditions and the boundary conditions of this work is that GBs in this work are assumed

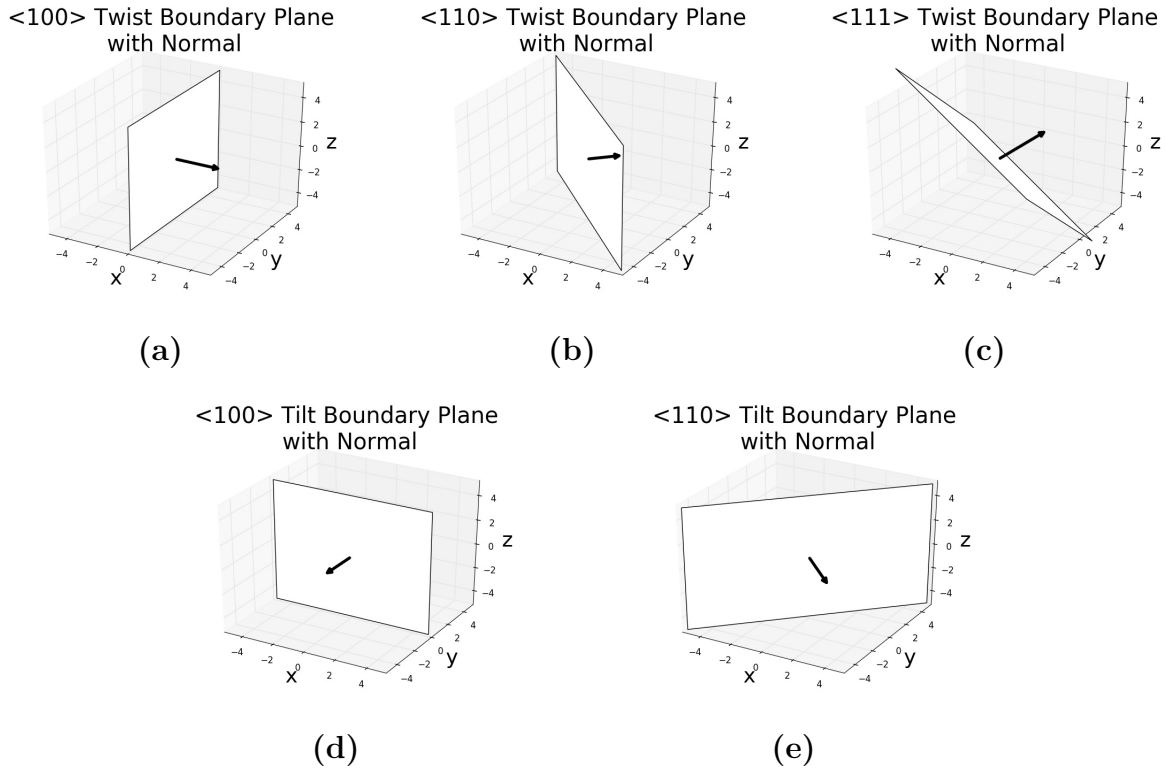


Figure 2.4 A geometric method of determining the normals of a GB. (a) to (c) show the GB normals for a GB perpendicular to the axis of rotation (a twist GB). The GB normal is simply the axis about which the grains are rotated. (d) and (e) show the GB normals for a GB parallel to the axis of rotation (a tilt GB). The GB normal is perpendicular to the axis of rotation. The same GB normal for ⟨110⟩ Tilt can be used for ⟨111⟩ Tilt.

to be either perpendicular or parallel to the rotation axis, as opposed to always being along the x- or y-axis.

The second method used an open-source MATLAB® package called MTEX.[19] This package calculates Euler angles using quaternions. These Euler angles did not generate the correct results either, for the most part creating the same sorts of graphs as the MARMOT method. It is uncertain why this method did not work.

The working method used the mathematics of quaternions directly.[20] The quaternions were calculated based on the misorientation axis and angle. A quaternion is a four-dimensional vector containing one real part, and three imaginary parts. The components of the vector

Table 2.1 Table of GB normals for different GB types. The normalized dot product of the axis with the GB normal is zero in all tilt cases and one in all twist cases. There are two options for the grain boundary normals of each subset because of inversion symmetries.

Axis	Boundary Type	GB Normal
$\langle 100 \rangle$	Tilt	$[010]$
		$[0\bar{1}0]$
$\langle 110 \rangle$	Tilt	$[1\bar{1}0]$
		$[\bar{1}10]$
$\langle 111 \rangle$	Tilt	$[1\bar{1}0]$
		$[\bar{1}10]$
$\langle 100 \rangle$	Twist	$[100]$
		$[\bar{1}00]$
$\langle 110 \rangle$	Twist	$[110]$
		$[\bar{1}\bar{1}0]$
$\langle 111 \rangle$	Twist	$[111]$
		$[\bar{1}\bar{1}\bar{1}]$

are calculated as follows:

$$\boldsymbol{q} = \left[\cos\left(\frac{\theta}{2}\right),\ a_x \sin\left(\frac{\theta}{2}\right),\ a_y \sin\left(\frac{\theta}{2}\right),\ a_z \sin\left(\frac{\theta}{2}\right)\right], \tag{2.6}$$

with axis $\boldsymbol{a}$ and misorientation angle θ. After converting the axis and misorientation angle to a quaternion, another conversion from a quaternion to the Bunge Euler angles is performed. The angles are calculated using the `atan2` method which allows for all four quadrants in the

Cartesian space to be accounted for. The angles are calculated using the following formulas:

$$\begin{aligned}
\chi &= \sqrt{(q_0^2 + q_3^2)(q_1^2 + q_2^2)} \\
\varphi_1 &= \text{atan2}\left(\frac{q_0 q_2 + q_1 q_3}{2\chi}, \frac{q_0 q_1 - q_2 q_3}{2\chi}\right) \\
\Phi &= \text{atan2}\left(2\chi, q_0^2 + q_3^2 - q_1^2 - q_2^2\right) \\
\varphi_2 &= \text{atan2}\left(\frac{q_1 q_3 - q_0 q_2}{2\chi}, \frac{q_0 q_1 + q_2 q_3}{2\chi}\right).
\end{aligned} \tag{2.7}$$

Once the Euler angles were calculated, they were put into Equation (2.3), and the resulting matrices were used as the orientation for the grains. The codes used to generate the orientation matrices can be found in Appendices D and F.

Testing The Matrices

This work attempted to reproduce the 1D subset graphs as shown in Bulatov *et al.* as a way to test the different methods. Various levels of success were observed for the different methods. The matrices giving the best results are shown in Figures C.1 to C.3.

While the first method works well for MARMOT, the challenge accompanying its use was that MARMOT specifies a specific GB normal with the set up of the problem that is not necessarily what the MATLAB® script expects. Thus, the results coming from using this combination of matrices ended up working only for the ⟨100⟩ tilt, ⟨110⟩ tilt, and ⟨100⟩ twist subsets. The ⟨110⟩ twist had issues with singularities, and the ⟨111⟩ subsets did not remotely match the expected outcome.

2.4.2 Calculating Reduced Chi Squared

There were two methods that this work used to calculate the χ^2_{red} statistic. The first method used the P and Q matrices as developed above to test the entirety of the fit. The second method calculated the statistic for each 1D subset, then calculated the full χ^2_{red} value using the statistics from the subsets. Results from these calculations are discussed in the next chapter.

The test for the entire fit used the P and Q matrices to calculate the energy in 1° intervals for each subset, using Bulatov *et al.*'s `GB5DOF.m` script. The χ^2_{red} value was calculated for each subset and for the entire fit using Equation (2.8), producing the results in Table 3.1 under the 800 K anneal column under the "χ^2_{red} using P and Q matrices" section.

$$\chi^2_{\text{red}} = \frac{1}{N-n-1} \sum \frac{(\epsilon_{\text{md}} - \epsilon)^2}{e\ \epsilon_{\text{md}}}. \tag{2.8}$$

In this equation, N is the number of observations, n is the number of parameters, ϵ_{md} are the energies from MD, ϵ are the energies from the model, and e is the uncertainty in the MD results.

Using the second method, the same angles used in the fitting procedure were used in the RSW equations creating the 1D subsets. The differences between the values resulting from there and the MD simulation values lead to the χ^2_{red} values shown in the 800 K anneal column under the χ^2_{red} comparing the 1D fits section. The same methods were implemented to calculate the χ^2_{red} values for the data without an anneal.

The statistic calculated using these methods is different from the χ^2 statistic used in the grid-search function. The grid search used Equation (2.9), and generated values of the same order as Equation (2.8).

$$\chi^2 = \sum (E_{\text{measured}} - E_{\text{calculated}})^2 \tag{2.9}$$

Chapter 3

Results and Discussion

3.1 Validation of P and Q Matrices

The energy profiles calculated from the P and Q matrices were compared with the copper energy profiles expected from the parameters defined in Bulatov *et al.*'s code to validate the generated P and Q matrices. Results from this comparison for the $\langle 100 \rangle$ set are shown in Figure 3.1, with all six subsets shown in Figures C.1 to C.3. The calculated energies match exactly the predicted values for all but a few points. Each data set does not match the expected energy at 1°, and the tilt data sets also see this mismatch at their second to last data point.

3.2 Fitting Results

Comparisons for the one-dimensional (1D) results from Harbison[4] and this work are presented in Figures 3.2 to 3.4. The results show a general decrease in the grain boundary (GB) energies, allowing trends in the different subsets to emerge. These trends allow for an all around better fit, but there are still some unexpected results present. The parameters calculated from the fitting procedure are shown in Appendix A.

Initial MD recalculations of the $\langle 100 \rangle$ symmetric tilt GB energies using the 800 K anneal

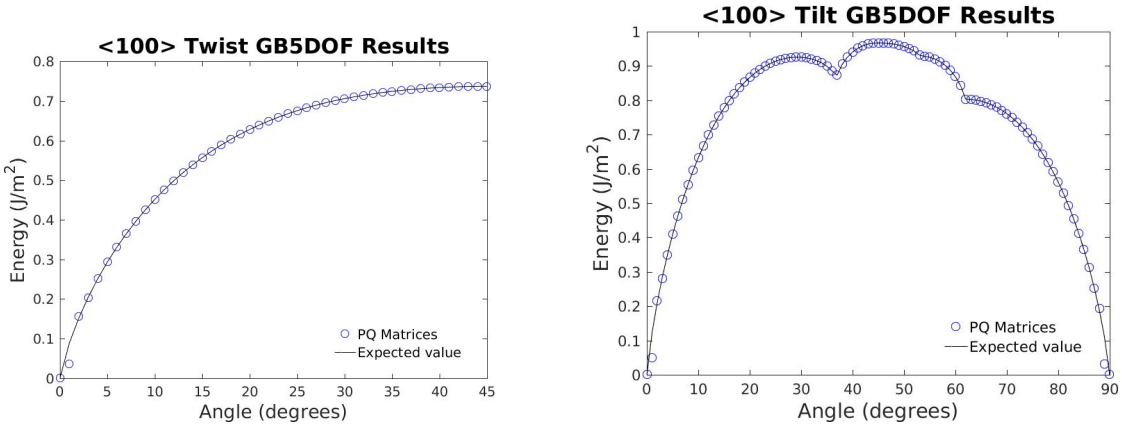


Figure 3.1 The ⟨100⟩ twist (a) and tilt (b) results for the P and Q matrices as compared to Bulatov *et al.*'s energy profiles. The expected value was calculated using Bulatov *et al.*'s `GB5DOF.m` MATLAB® script with the default values. The calculated values were found by inputting the matrices into the `GB5DOF.m` script. With the exception of the data points at 1° in both (a) and (b) and 89° in (b), the energies calculated from the matrices matches the expected curves exactly.

(Figure 3.2b) showed an unexpected deep cusp around 28°. An analysis of the molecular dynamics (MD) simulation results for this misorientation revealed that, in this case, the two crystals had realigned during the simulation due to abnormally high pressures. This realignment caused the misorientation angle to change causing the GB energy to be much lower than expected. Comparison with Harbison's simulation result revealed that the crystal structure from his simulation did not realign. While Harbison's data was not calculated with the anneal and thus may not represent a global minimum, the data point follows the surrounding data's trend, justifying the use of his result.

Of the symmetric tilt GB energy sets, the ⟨110⟩ set has the most improvement. All three sets showed a general decrease in the energy, increasing confidence in the accuracy of the fit for GB energies in uranium dioxide (UO_2). However, each of these sets provides more opportunity for research. The ⟨100⟩ set needs more work done for data points after around 50°. The scatter associated with those points seems to be higher, and the possibility of a slight cusp presents itself around 68°. It is unknown what behaviors are expected there

though because of the limited data in that region, so additional data would prove beneficial. The ⟨110⟩ set as mentioned shows the most improvement, but some low points in the second and third "humps" do not follow the trend, indicating further possibility for cusps. The first part of the function (the first hump) needs additional data to determine the possibility of a cusp between 40° and 50°. The fitted curve to the ⟨111⟩ set now has an unexpected upward trend. The relatively high scatter associated with these data points leads to the possibility of a completely different set of functions to define this subset, meaning additional RSW functions would be required for example.

The twist GB energy sets vary in their success. The ⟨100⟩ set shows little difference between Harbison's[4] work and this work. An unexpected slight positive concavity at the end of the fitting for this subset indicates the possibility of a cusp. This cusp may occur around 30°. The ⟨110⟩ set has a definite decrease in the overall energies, creating a plateau profile. An additional cusp around 40° is being considered. The ⟨111⟩ set has the least improvement. From the Bulatov *et al.*'s work[9] this work expected to see a plateau as Harbison's fitting demonstrated.[4] Instead, the fitting produced a curved energy profile, indicating the potential for at least one cusp. A possible location of this cusp is around 35°. Preliminary work has been done with changing the number of parameters in an effort to maximize the quality of the fit with a minimal number of parameters. Figure 3.6 compares the current fitting to the tentative new fitting for three of the six 1D subsets. These modified fits in general seem to fit better at the cost of additional parameters, with a smaller χ^2_{red} value. Still more parameters may be needed to accommodate additional cusps however.

Figure 3.5 shows the comparison between the values calculated from the P and Q matrices and the expected values from the MD calculations for the ⟨100⟩ subset. All six subsets are shown in Figures C.4 to C.6 in Appendix C. There is an unsolved scaling issue with the ⟨100⟩ tilt subset. Overall, the results from the P and Q matrices match the fitted values, with a few anomalies needing to be addressed.

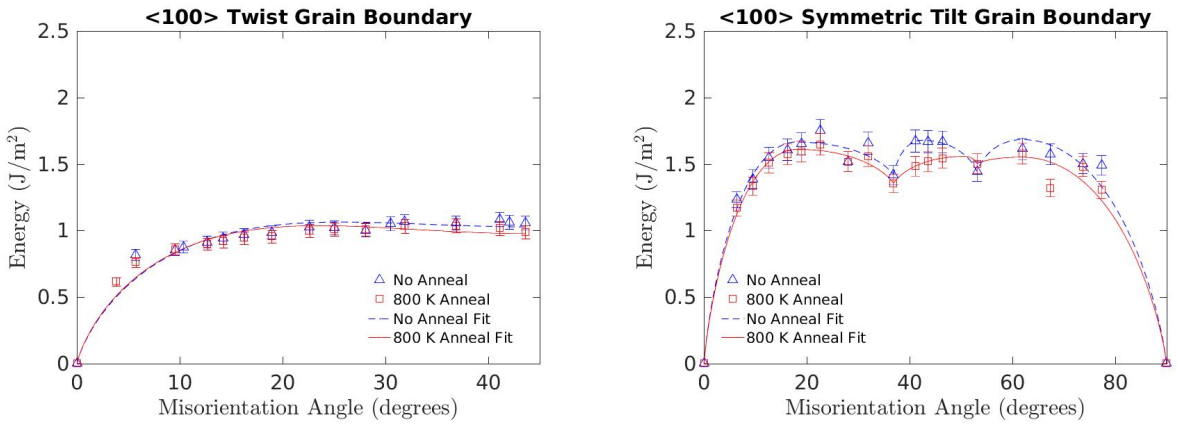


Figure 3.2 The ⟨100⟩ twist (a) and tilt (b) results. In general the re-calculated energies are lower, with significant differences around 40° to 50° in the tilt subset. The positive concavity in the twist subset around 40° is unexpected, and may indicate the presence of a missing cusp. There is a possible cusp around 30° in the twist subset, and around 68° in the tilt subset.

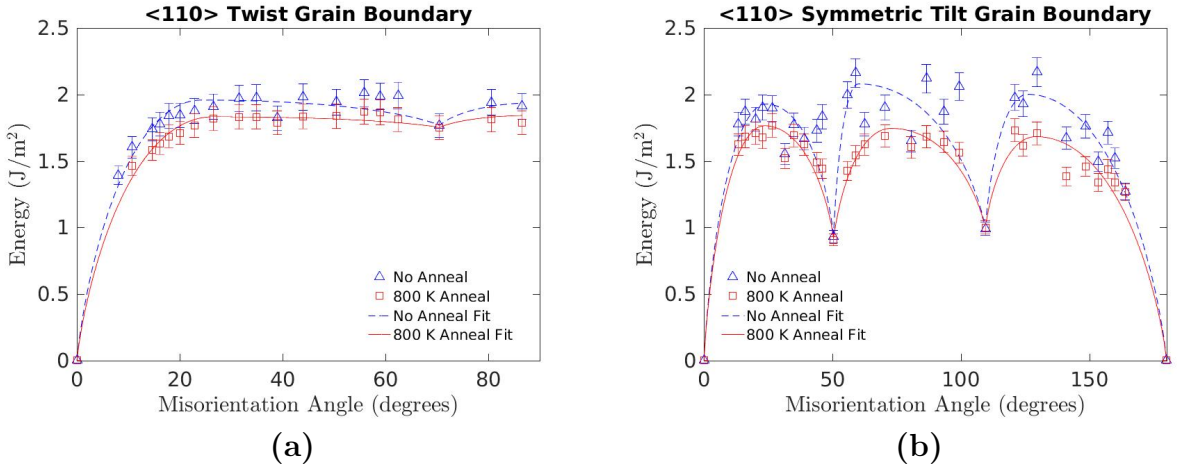


Figure 3.3 The ⟨110⟩ twist (a) and tilt (b) results. Significant decreases in energy are found for both subsets. Possible cusp locations are around 40° in the twist subset, and around 40°, 90°, and 140° in the tilt subset.

3.3 Reduced Chi-square Results

The χ^2_{red} values are much smaller than one for every data set regardless of the method used to calculate the statistic, with the exception of the ⟨100⟩ symmetric tilt subset using the P and Q matrices. This subset has a high χ^2_{red} value due to the scaling issue. Because of the

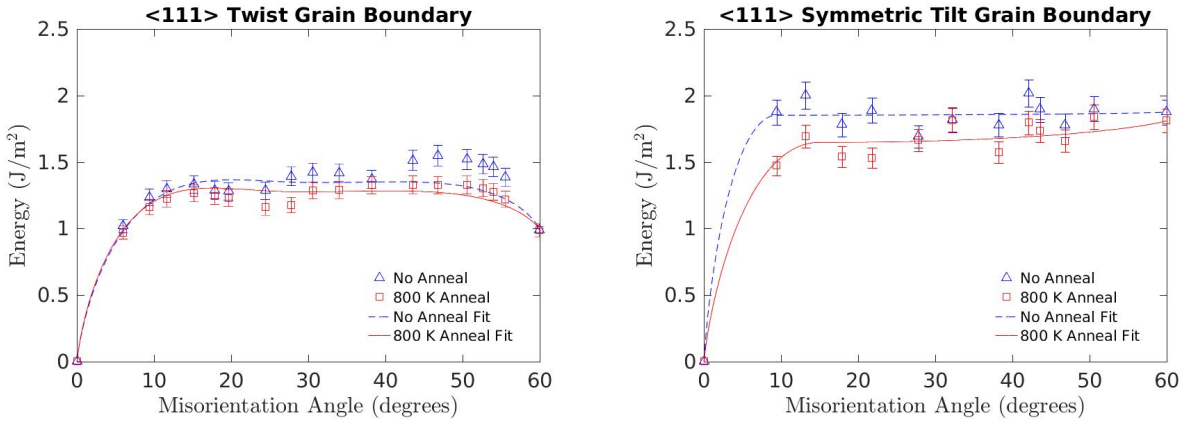


Figure 3.4 The ⟨111⟩ twist (a) and tilt (b) results. Some energies are found to be lower, but some are found to be higher. The positive concavity present in these results is unexpected, and could indicate the presence of cusps. A possible location for the twist subset is around 33°. Additional data is needed to determine possible cusp locations for the tilt subset.

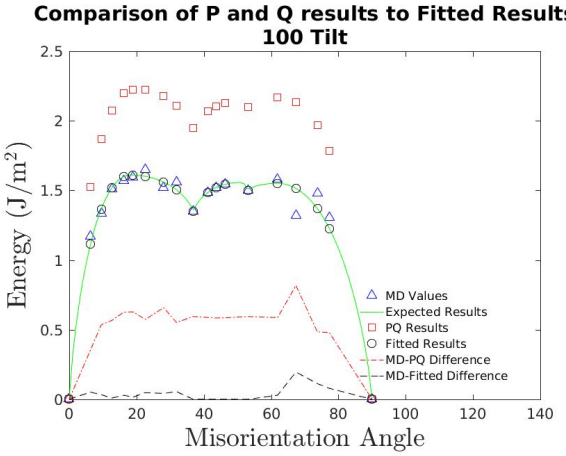


Figure 3.5 A comparison of the expected value of the fitted function with the values calculated using the P and Q matrices for the ⟨100⟩ 1D tilt subset. The MD values are shown for reference. There is a scaling issue yet to be fixed, but it is uncertain what causes the scaling issue for this subset.

low χ^2_{red} values, the fitted functions overfit the data.[16] Table 3.1 lists the χ^2_{red} values for the 1D subsets using the two different methods for calculation.

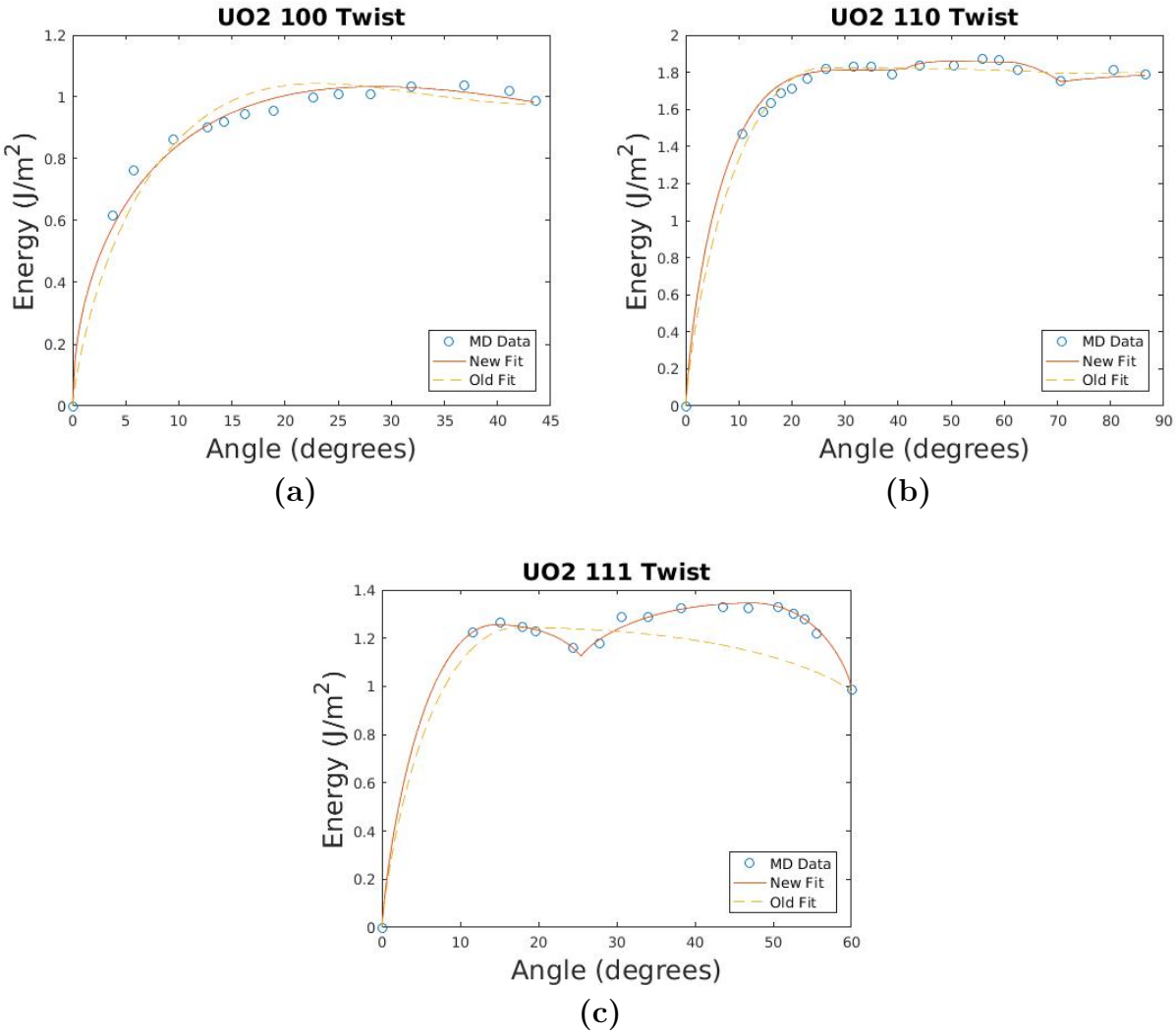


Figure 3.6 A comparison of current fitting functions with a possible change to the functions. Original functions are shown as the dashed lines, with the updated functions shown as the solid lines. MD results are shown for reference. (a) shows a possible change from the Read-Shockley-Wolf (RSW) functions to a simple square root function multiplied by an exponential decay. There is no theoretical basis behind this change however. (b) attempts to fit to a cusp around 40°. Further work can be done to find a better fit for this subset. (c) shows the most potential improvement. The potential fit increases the total number of parameters by three to fit to the cusp around 28°. A quick glance at the MD values compared to the fit shows a great improvement from the current fit. To create the graph shown in (c) two additional RSW functions were spliced into the original function. This created a total of four RSW functions for this subset.

Table 3.1 A list of the χ^2_{red} results using two different methods: using the P and Q matrices for the various orientations to test the fit, and comparing the results of the 1D fits to the 1D data. The values for χ^2_{red} are all less than one with the exception of the $\langle 100 \rangle$ symmetric tilt using the P and Q matrices. These values indicate an over-fit to the data.

1D Subset	χ^2_{red} using P and Q matrices		χ^2_{red} comparing the 1D fits	
	No Anneal	800 K Anneal	No Anneal	800 K Anneal
$\langle 100 \rangle$ Twist	0.0953	0.1074	0.0752	0.0722
$\langle 110 \rangle$ Twist	0.1010	0.1874	0.0400	0.0137
$\langle 111 \rangle$ Twist	0.3041	0.1139	0.4966	0.1516
$\langle 100 \rangle$ Tilt	0.1038	8.7702	0.0846	0.0932
$\langle 110 \rangle$ Tilt	4.9799	0.3277	0.5951	0.1762
$\langle 111 \rangle$ Tilt	0.1566	0.7814	0.1315	0.1355
Overall χ^2_{red}	1.7652	1.4893	0.2678	0.1153

Chapter 4

Conclusion

This work has successfully created a more accurate interpolation function for grain boundary (GB) energies in uranium dioxide (UO_2), but additional characteristics of the full five-dimensional (5D) GB space have been revealed that require further research. GB energies were found to be lower when calculated with an 800 K anneal as expected when compared to the data set created without an anneal. Descriptions of those additional characteristics through the use of additional functions will prove beneficial.

The most important work yet to be done is calculation of additional data points for fitting. Increasing the number of data points will improve the quality of the fit. Additional data points will also help to identify trends that do not readily appear with the limited data currently available. The difficulty associated with calculating additional data points is the required computational resources.

Further work could generalize this function to all polycrystalline materials with the fluorite crystal structure. Such a generalization would provide further validation of this model, however, such validation would require a sufficient number of GB energies for many different materials with such a structure. As these energies are not already available in the literature, this would require additional computational resources. As the parameters for GB energy interpolation are improved and validated, they should be incorporated into MARMOT to

further the anisotropic grain growth model being developed.

As the model is developed, initial conditions set by actual nuclear fuel data will be put into a MARMOT simulation. After simulating grain growth in a nuclear reactor, the fuel data will be compared with the simulation data to determine the accuracy of the model.

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Appendix A

List of Parameters

Table A.1 This table gives the parameters for UO_2 generating the energy function.

Array number	Parameter name	Parameter value
1	Energy Scaling Factor (e_{RGB})	1.6012 J/m^2
2	$\langle 100 \rangle$ Max Distance	0.405
3	$\langle 110 \rangle$ Max Distance	0.739
4	$\langle 111 \rangle$ Max Distance	0.352
5	$\langle 100 \rangle$ Weight	50.5
6	$\langle 110 \rangle$ Weight	4.55
7	$\langle 111 \rangle$ Weight	0.08
8	$\langle 100 \rangle$ Tilt/Twist Mix Power Law (1)	0.03325
9	$\langle 100 \rangle$ Tilt/Twist Mix Power Law (2)	0.00053125
10	Maximum $\langle 100 \rangle$ Twist Energy	0.60903
11	$\langle 100 \rangle$ Twist Shape Factor	1.4486
12	$\langle 100 \rangle$ Asymmetric Tilt Interpolation Power	35.8
13	$\langle 100 \rangle$ Symmetric Tilt First Peak Energy	1.0058

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Table A.1 – *Continued from previous page*

Array number	Parameter name	Parameter value
14	⟨100⟩ Symmetric Tilt First Σ5 Energy	0.84456
15	⟨100⟩ Symmetric Tilt Second Peak Energy	0.97259
16	⟨100⟩ Symmetric Tilt Second Σ5 Energy	0.9379
17	⟨100⟩ Symmetric Tilt Σ17 Energy	0.96881
18	⟨100⟩ Symmetric Tilt First Peak Angle	0.31569
19	⟨100⟩ Symmetric Tilt Second Peak Angle	0.88538
20	⟨110⟩ Tilt/Twist Mix Power Law (1)	3.1573
21	⟨110⟩ Tilt/Twist Mix Power Law (2)	1.9784
22	⟨110⟩ Twist Peak Angle	0.46145
23	⟨110⟩ Twist Peak Energy	1.1444
24	⟨110⟩ Twist Σ3 Energy	1.0931
25	⟨110⟩ Twist 90° Energy	1.152
26	⟨110⟩ Asymmetric Tilt Shape Factor	3.1843
27	⟨110⟩ Symmetric Tilt Third Peak Energy	1.0514
28	⟨110⟩ Symmetric Tilt Σ3 Energy	0.61703
29	⟨110⟩ Symmetric Tilt Second Peak Energy	1.0902
30	⟨110⟩ Symmetric Tilt Σ11 Energy	0.56686
31	⟨110⟩ Symmetric Tilt First Peak Energy	1.1024
32	⟨110⟩ Symmetric Tilt Third Peak Angle	0.88736
33	⟨110⟩ Symmetric Tilt Second Peak Angle	1.8711
34	⟨110⟩ Symmetric Tilt First Peak Angle	2.731
35	⟨111⟩ Tilt-Twist Linear Interpolation	38.201
36	⟨111⟩ Twist Shape Factor	1.2414
37	⟨111⟩ Twist Peak Angle	0.49979

Continued on next page.

Table A.1 – *Continued from previous page*

Array number	Parameter name	Parameter value
38	⟨111⟩ Twist Peak Energy	0.7971
39	⟨111⟩ Symmetric Tilt Peak Angle	0.25966
40	⟨111⟩ Symmetric Tilt Max Energy	1.0288
41	⟨111⟩ Symmetric Tilt Σ3 Energy	1.1311
42	⟨111⟩ Asymmetric Tilt Symmetry Point Energy	3.7674
43	⟨111⟩ Asymmetric Tilt Scale Factor	0.053417

Appendix B

Grain Boundary Representations

Part of Bulatov *et al.*'s development of their 5D function was accomplished through visual representations of the GB space. However, the size of the five-space in which GBs reside makes representing them difficult. Different methods have been developed to represent them, each with their advantages and disadvantages. Three of these methods are the axis-angle representation, the Rodrigues representation, and the fundamental zone representation. These methods, though described separately, can be used together to form a better picture of what the GB space looks like (see for example Figure 2.2b which combines the Rodrigues representation and the fundamental zone representation).

B.1 Axis-Angle Representation

The axis-angle representation is the simplest of the three described here. The axis of rotation of the GB specifies the point in axis-angle space, and the angle of misorientation between the two grains at the GB specifies the magnitude of the vector. Thus, the axis ($\boldsymbol{a}$, where $\boldsymbol{a}$ has components a_x, a_y, and a_z) and the angle (θ) mathematically represent an axis-angle vector as:

$$\boldsymbol{A} = \boldsymbol{a}\ \theta \tag{B.1}$$

The axis-angle space can only take into account three degrees of freedom: the two angles specifying the axis, and the angle rotated through. Thus, axis-angle space cannot fully visualize all of the necessary information contained in the full 5D space.[21] An added difficulty of using this representation is its infinite space because it maps an axis and an angle onto a Cartesian coordinate system. This mapping means understanding the entire GB space is difficult without the help of additional methods. The axis-angle representation is best used as a starting point to move to other, more robust representations, and to represent the misorientation between two grains.[15]

B.2 Rodrigues Representation

The Rodrigues representation (sometimes called the "Rodrigues-Frank" representation) uses Rodrigues vectors to represent rotations in Rodrigues space. This representation takes ideas from the axis-angle space, but makes a few changes allowing crystal symmetries to be taken into account. The axis about which a GB is oriented still specifies the point in space, but the tangent of half the angle represents the magnitude of the vector. Thus, a Rodrigues vector can be represented as:[15,21–24]

$$\boldsymbol{R} = \boldsymbol{a} \tan\left(\frac{\theta}{2}\right) \tag{B.2}$$

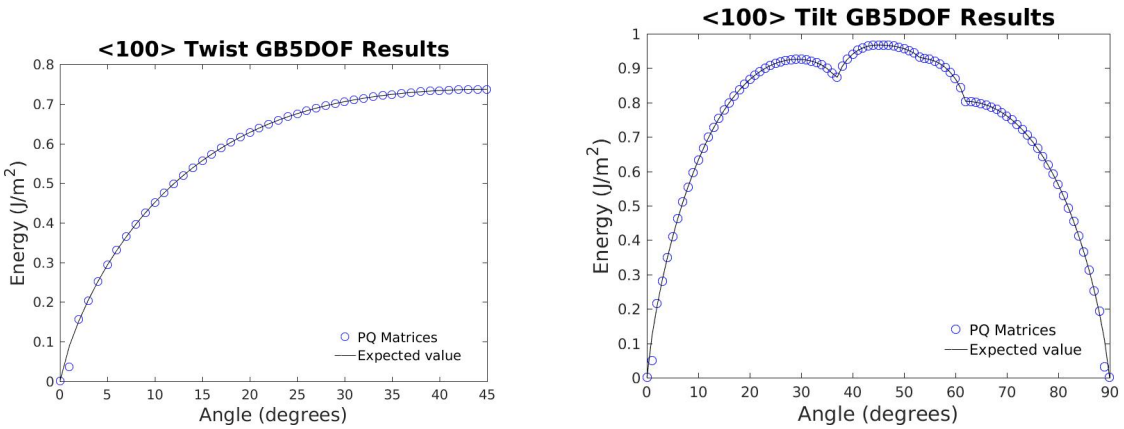
Some researchers favor this representation over others because of the lack of curvature such a mapping entails.[15,21] However, still only three of the five degrees of freedom are specified. Bulatov *et al.* attached a unit vector at the points along the axis to represent the other two DoFs in Figure 2.2b. A parallel vector represents a twist boundary, and a perpendicular vector represents a tilt boundary. Anything else represents a mix of twist and tilt (or a mixed boundary). One difficulty in using Rodrigues space is it also is an infinite space, as it also transforms an axis-angle pair into a Cartesian coordinates.[21,25]

B.3 Fundamental Zone Representation

The fundamental zone is perhaps the best graphical representation for the 5D GB. This representation takes advantage of the symmetries inherent in crystals[13] to simplify an infinite space into a compact, finite area called the fundamental zone.[6,8,9,22,26] Every point within the space represents a unique orientation, and every point outside the space can be represented as a point inside the space through symmetry operations.[21–23] Bulatov *et al.* used this idea in connection with Rodrigues space to create Figure 2.2b. In Rodrigues space, the crystal symmetries of the material determine the shape of the fundamental zone.[6,22] For fcc crystals, the fundamental zone takes the form of a truncated tetrahedron.[9] The edges of the fundamental zone in Rodrigues space represent the high-symmetry rotation axes, and points on one face can represent another point on a different face of the fundamental zone.

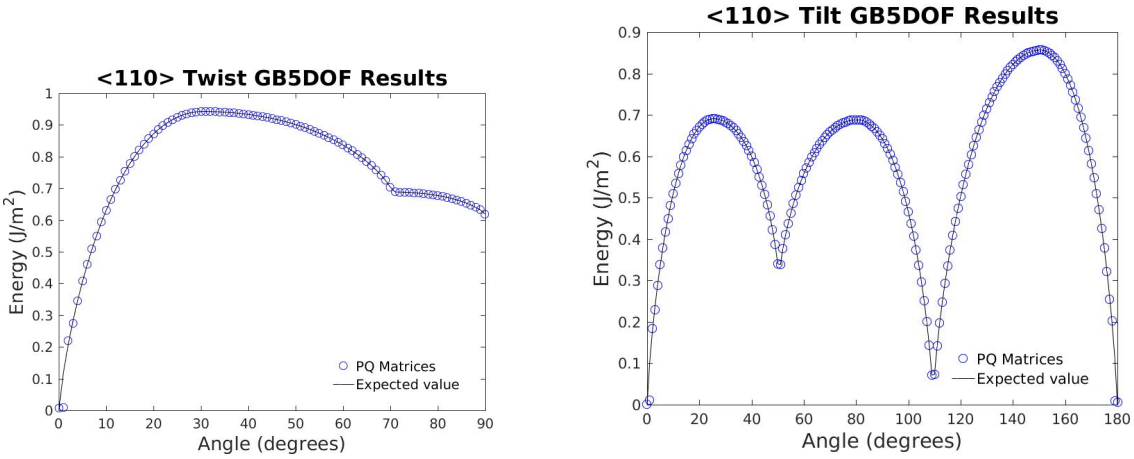
Appendix C

Graphs



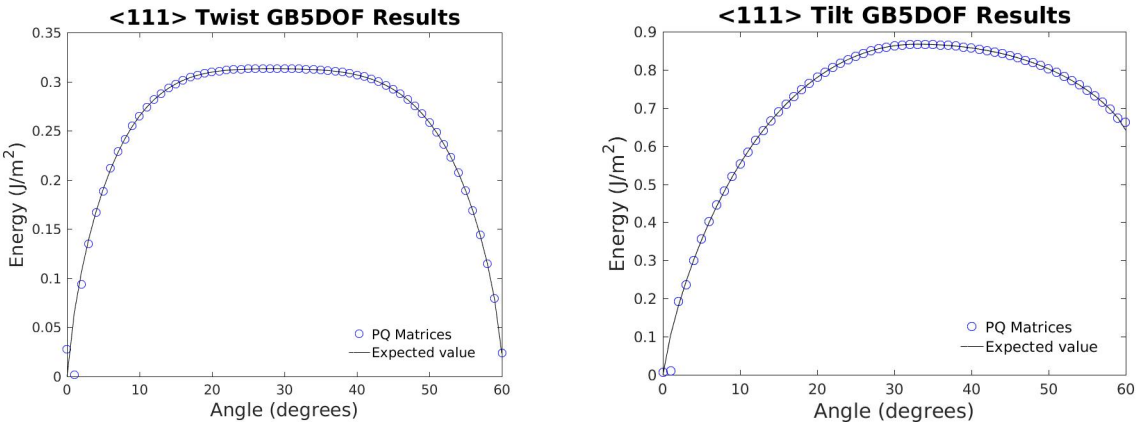
(a) **(b)**

Figure C.1 The ⟨100⟩ twist (a) and tilt (b) results for the P and Q matrices as compared to Bulatov *et al.*'s energy profiles. The expected value was calculated using Bulatov *et al.*'s `GB5DOF.m` MATLAB® script with the default values. The calculated values were found by inputting the matrices into the `GB5DOF.m` script. With the exception of the data points at 1° in both (a) and (b) and 89° in (b), the energies calculated from the matrices matches the expected curves exactly.



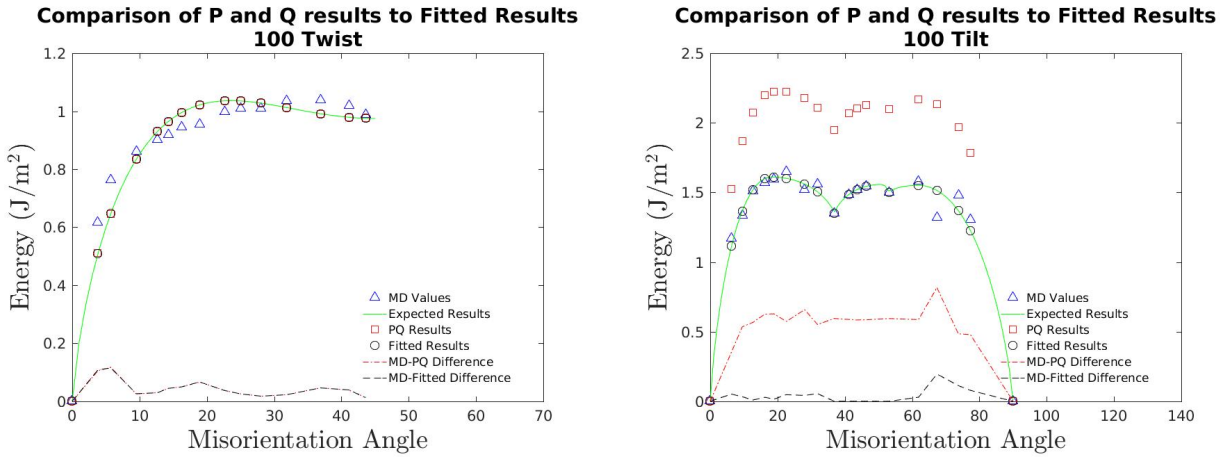
(a) **(b)**

Figure C.2 The ⟨110⟩ twist (a) and tilt (b) results for the P and Q matrices as compared to Bulatov *et al.*'s energy profiles. The expected value was calculated using Bulatov *et al.*'s `GB5DOF.m` MATLAB® script with the default values. The calculated values were found by inputting the matrices into the `GB5DOF.m` script. With the exception of the data points at 1° in both (a) and (b) and 179° in (b), the energies calculated from the matrices matches the expected curves exactly.



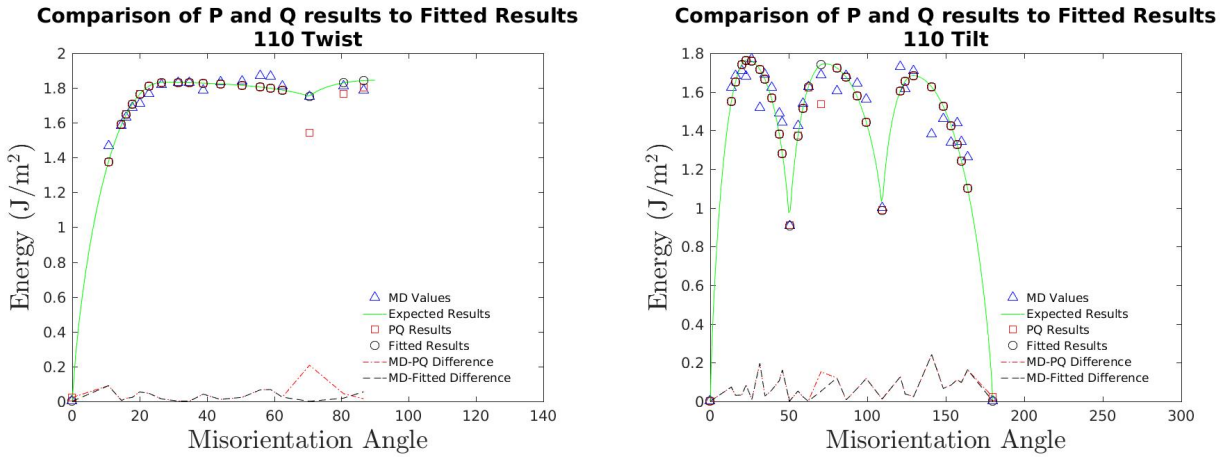
(a) **(b)**

Figure C.3 The ⟨111⟩ twist (a) and tilt (b) results for the P and Q matrices as compared to Bulatov *et al.*'s energy profiles. The expected value was calculated using Bulatov *et al.*'s `GB5DOF.m` MATLAB® script with the default values. The calculated values were found by inputting the matrices into the `GB5DOF.m` script. With the exception of the data points at 1° in both (a) and (b) and 60° in (b), the energies calculated from the matrices matches the expected curves exactly.



(a) **(b)**

Figure C.4 A comparison of the expected value of the fitted function with the values calculated using the P and Q matrices for the ⟨100⟩ 1D subsets. The MD values are shown for reference. (a) PQ results follow exactly the fitted curve. (b) has a scaling issue yet to be fixed. It is uncertain what causes the scaling issue for this subset.



(a) **(b)**

Figure C.5 A comparison of the expected value of the fitted function with the values calculated using the P and Q matrices for the ⟨110⟩ 1D subsets. MD values are shown for reference. (a) follows the fitted result until the cusp, at which point some anomalies appear. The results from the PQ matrices dip well below the expected value at the cusp, and never make it back to the original fitted line. (b) has a similar issue on a lesser scale. Only two of the calculated points do not follow the fitted curve. The endpoint is expected to return a zero value, where the PQ matrices calculated a value slightly higher. There is also an unexpected cusp from the PQ matrices in the middle of the second hump. All other data points follow the fitted curve exactly.

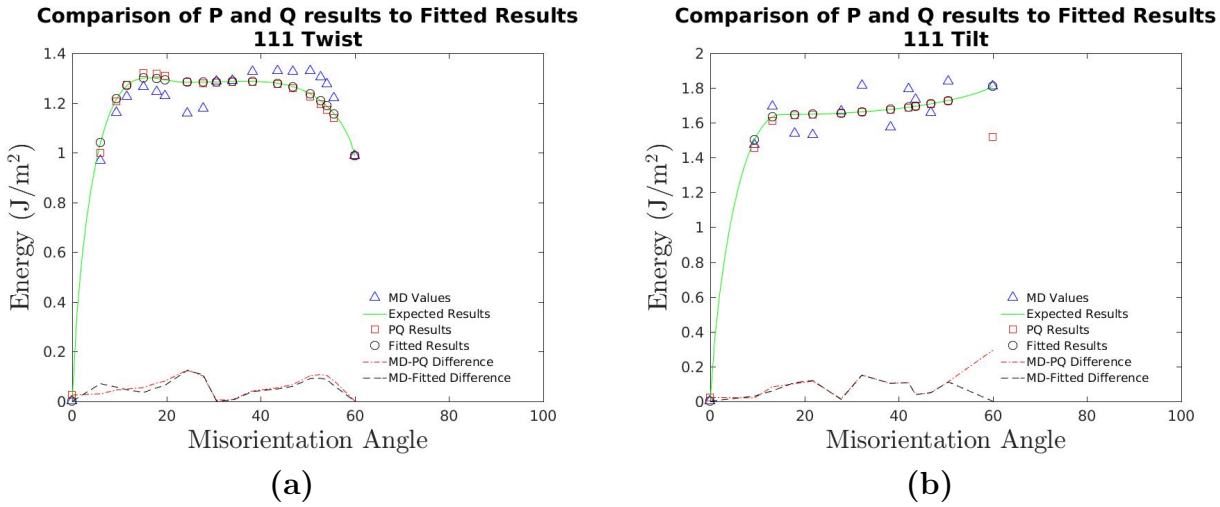


Figure C.6 A comparison of the expected value of the fitted function with the values calculated using the P and Q matrices for the ⟨111⟩ 1D subsets. MD values are shown for reference. (a) closely follows the expected fitted values, but has a slight error throughout. (b) follows the expected values exactly in the center of the fitting, but misses slightly for lower angle boundaries, and misses completely at the end.

Appendix D

Orientation Matrix Generator

This code generates the orientation matrices (known as the P and Q matrices in Bulatov *et al.*'s code). Provision for calculating the matrices one of two ways is provided in-code through the use of command-line options.

```
from __future__ import division,print_function # To avoid numerical
    problems with division, and for ease of printing
from sys import argv # for CLI arguments
from math import cos, sin, pi, atan2, sqrt # Trig functions
from os.path import exists # For checking existence of a file
from numpy import array, linalg
from myModules import * # imports my functions from the file myModules.py

# Helper functions
def displayHelp():
    print('''
    This script will calculate the orientation matrices for any given
        misorientation
    for any of the high-symmetry axes.
    Arguments:

        _axis: The axis of orientation (type: int)
```

```
16          _misorientation: The angle of misorientation (type: float)
                --------OR--------
18          (with option -e or --euler)
            _z1: The first rotation angle  (Z ) (type: float)
20          _x:  The second rotation angle (X') (type: float)
            _z2: The third rotation angle  (Z") (type: float)
22
        If the option -e or --euler-angles is entered, the calculation skips
            to simply
24      output the orientation matrices.  Otherwise, the Euler angles are
            calculated from
        the axis, orientation, and grain boundary normal, and then the
            orientation matrix is
26      created through the use of the Rodrigues Rotation Formula, which is:
        R = I + sin(theta) * K + (1 - cos(theta))*K^2
28      where I is the identity matrix, theta is the misorientation angle, and
             K is
        the skew-symmetric matrix formed by the axis of rotation:
30      K = 0  -kz  ky
             kz  0  -kx
32          -ky  kx  0
        where the vector k is the unit vector defining the axis of rotation,
            or using
34      a set of predefined rotations for each axis (default is the predefined
             rotations).
        The Euler angles are calculated in this case simply for the file to be
             written
36      to.  If the user does not specify to save, then the angles are not
            used for
        anything.
38
        Options:
```

```
40      -e --euler <_z1> <_x> <_z2>          Returns the  Bunge orientation
          matrix
                                             based on the euler angles provided
                                                .
42
        -f --file <filename>                 Reads the file filename and uses
          the
44                                           Euler angles from them to
                                                calculate the
                                             orientation matrix.
46
        --rrf                                Calculates the matrices using the
          Rodrigues
48                                           Rotation Formula

50      -a --angles                          Displays the Euler angles.  Can be
           used
                                             in conjunction with -q or --quiet
                                                to
52                                           display only the Euler angles.

54      -s --save                            Saves the resultant orientation
          matrix to
                                             a database (
                                                orientation_matrix_database.m)
56                                           with the accompanying Euler angles
                                                .

58      -q --quiet                           Suppresses output of the
          orientation matrices
                                             to the terminal
60
```

```
        --help                                  Displays this help info
62
        Output:
64      For an Euler angle set, the ouput is simply its orientation matrix.
        For the misorientations, the first matrix is the 'P' orientation
            matrix, and
66      the second matrix is the 'Q' orientation matrix (see Bulatov et al.,
            Acta Mater
        65 (2014) 161-175).
68      ''')
        return
70
    def displayAngles(z1, x, z2): # Displays an Euler angle set (Bunge
        convention)
72      print("Euler angles:")
        # This is the "new" way to format strings.  The 16 indicates the
            padding to
74      # be done before the next character.  The '<' character below says
            which side
        # to pad (the right side).
76      print("{:16}{:16}{:16}".format('Z', 'X', 'Z'))
        print("----------------------------------------")
78      print("{:<16}{:<16}{:<16}\n".format(rad2deg(z1), rad2deg(x), rad2deg(
            z2)))
        return
80
    def check4RRF(args): # Check the args for the rrf command
82      if "--rrf" in args:
            index = args.index("--rrf")
84          del args[index]
            return True, args
86      else:
```

```
        return False, args

def check4Euler(args): # Check the args for the -a or --angles command
    if "-a" in args or "--angles" in args:
        try:
            index = args.index("-a")
        except:
            index = args.index("--angles")
        del args[index]
        return True, args
    else:
        return False, args

# Write the matrix and angles to a file
def writeMat(m, _z1, _x, _z2, grain, axis):
    # This is to avoid issues with duplicates
    if _z1 == 0:
        _z1 = abs(_z1)
    if _x == 0:
        _x = abs(_x)
    if _z2 == 0:
        _z2 = abs(_z2)

    lastVal = 1
    # This is the default filename to be used.
    # TODO: make provisions to provide the database file via command line
    tex_filename = "orientation_matrix_database.m"
    var_name = "%s%d"%(grain, axis) # Will generally look like P100 or
       Q100
    if not exists(tex_filename):
        tex_file = open(tex_filename, "a")
```

```
        tex_file.write("%Database for orientation matrices for specified
            Euler Angles\n")
118     tex_file.write("
            %--------------------------------------------------------------\
            n")
        tex_file.write("%Orientation Matrix
                                                Euler Angles\n")
120     tex_file.write("%s(:,:,%d)=[%2.6f  %2.6f  %2.6f           %%%2.4f
             %2.4f  %2.4f\n"%(var_name, lastVal, m[0][0], m[0][1], m[0][2],
             _z1, _x, _z2))
        tex_file.write("%2.6f  %2.6f  %2.6f\n"%(m[1][0], m[1][1], m[1][2])
            )
122     tex_file.write("%2.6f  %2.6f  %2.6f];\n"%(m[2][0], m[2][1], m
            [2][2]))
        tex_file.write("
            %--------------------------------------------------------------\
            n")
124     tex_file.close()
    else:
126     f = open(tex_filename,"r")
        while True:
128         data = f.readline().split()
            if not data:
130             break
            elif len(data) != 6:
132             continue
            else:
134             assert data[0][0] in {'P', 'Q'}, "Unknown orientation
                    matrix type (should be \'P\' or \'Q\')."
                if not "%d"%(axis) in data[0][1:4]:
136                 lastVal = 0
                elif "%d"%(axis) in data[0][1:4]:
```

```
                    try:
                        try:
                            if data[0][0] == 'P': # Handles anything 3
                                digits long
                                lastVal = int(data[0][9:12]) - 1
                            else:
                                lastVal = int(data[0][9:12])
                        except:
                            if data[0][0] == 'P': # Handles anything 2
                                digits long
                                lastVal = int(data[0][9:11]) - 1
                            else: # data[0][0] == 'Q'
                                lastVal = int(data[0][9:11])
                    except:
                        if data[0][0] == 'P': # One digit case
                            lastVal = int(data[0][9]) - 1
                        else: # data[0][0] == 'Q'
                            lastVal = int(data[0][9])
                else:
                    print("Error: Unknown last index.")
                    exit()

                # Checks to see if the Euler angles have already been used
                    before
                # If so, the calculated matrix is not saved (assumed to
                   already
                # be in the database)
                if data[0][0] == grain and data[3] == ('%' + "%2.4f"%_z1)
                   and data[4] == "%2.4f"%_x and data[5] == "%2.4f"%_z2:
                    unique = False
                    break
                else:
```

```
                    unique = True
166         if unique:
                tex_file = open(tex_filename, "a")
168             tex_file.write("%s(:,:,%d)=[%2.6f  %2.6f  %2.6f
                    %%%2.4f  %2.4f  %2.4f\n"%(var_name, lastVal + 1, m[0][0], m
                    [0][1], m[0][2], _z1, _x, _z2))
                tex_file.write("%2.6f  %2.6f  %2.6f\n"%(m[1][0], m[1][1], m
                    [1][2]))
170             tex_file.write("%2.6f  %2.6f  %2.6f];\n"%(m[2][0], m[2][1], m
                    [2][2]))
                tex_file.write("
                    %-------------------------------------------------------------------\
                    n")
172             tex_file.close()
        return
174
    if "--help" in argv: # Help info
176     displayHelp()
        exit()
178
    orientation_matrix = []
180 save, argv = check4Save(argv) # Save the file?  Delete the save argument
    quiet, argv = check4Quiet(argv) # Checks for suppressing output. Delete
        the quiet argument.
182 useRRF, argv = check4RRF(argv) # Checks for using the RRF method. Delete
        the rrf argument.
    dispEuler, argv = check4Euler(argv) # Checks for displaying the Euler
        angles.  Delete the angle argument
184
    # If the arguments come from a file...
186 if "-f" in argv or "--file" in argv: #input arguments come from file
        try:
```

```
188         try:
                index = argv.index("-f")
190         except:
                index = argv.index("--file")
192     except:
            print("ERROR: Unable to find filename.")
194         exit()
        filename = argv[index + 1]
196     try:
            f1 = open(filename, 'r')
198     except:
            print("ERROR: Unable to read file.", filename)
200
        while True: # Read the file line by line.
202         line = f1.readline()
            # break if we don't read anything.  If there are blank lines in
               the
204         # file, this will evaluate to TRUE!
            if not line:
206             break;
            data = line.split()
208         if len(data) != 4: # If there are less than 4 parts to the data,
               move along (format of file MUST be _z1 _x _z2 1.00)
                continue
210         else:
                # Convert the data to stuff we can use
212             _z1 = float(data[0])
                _x  = float(data[1])
214             _z2 = float(data[2])

216             _z1 = deg2rad(_z1)
                _x  = deg2rad(_x)
```

```
218             _z2 = deg2rad(_z2)
                orientation_matrix = calcRotMat(_z1, _x, _z2)
220             if not quiet:
                    displayMat(orientation_matrix)
222             if save:
                    writeMat(orientation_matrix, _z1, _x, _z2,'P', _axis)
224
# Input is a set of euler angles
226 elif "-e" in argv or "--euler-angles" in argv:
    try:
228         try:
                index = argv.index("-e")
230         except:
                index = argv.index("--euler-angles")
232     except:
            print("ERROR: Unable to read Euler angles.")
234         exit()
        _z1 = float(argv[index + 1])
236     _x =  float(argv[index + 2])
        _z2 = float(argv[index + 3])
238     _z1 = deg2rad(_z1)
        _x  = deg2rad(_x)
240     _z2 = deg2rad(_z2)

242     orientation_matrix = calcRotMat(_z1, _x, _z2)

244     if not quiet:
            displayMat(orientation_matrix)
246     if save:
            writeMat(orientation_matrix, _z1, _x, _z2, 'P', _axis)
248
else:
```

```
250     if len(argv) < 3:
            print("ERROR: Not enough command line arguments.")
252         print("Input either an axis, and a misorientation, or a ZXZ Euler
                angle set with the option -e or --euler-angles.")
            displayHelp()
254         exit()
        try:
256         _axis = int(argv[1])
            _misorientation = float(argv[2])
258     except:
            print('''
260         ERROR: Command line argument(s) is (are) not of correct type.
            Please enter an int for argument 1, a float for argument 2, and an
                int for argument 3.
              ''')
            exit()
264
        if not len(str(_axis)) == 3: # axis length greater than 3
266         print("ERROR: Argument 1 must by a 3 digit number like \'100\'.")
            exit()
268
        _misorientation = deg2rad(_misorientation) # Change input to radians
270     axis = [None]*3
        _z1 = [None]*2
272     _x = [None]*2
        _z2 = [None]*2
274     q = [None]*2
        for i in range(0, len(str(_axis))):
276         axis[i] = int(str(_axis)[i])

278 #
    ------------------------------------------------------------------------#
```

```
#------------------------------The Actual Calculations
    ------------------------#
#
    ------------------------------------------------------------------------------#

    # First convert to a quaternion
    # These functions are from a myModules.py.
    q[0] = axis2quat(axis, _misorientation / 2)
    q[1] = axis2quat(axis, -_misorientation / 2)

    # Convert the quaternion to Euler Angles
    for i in range(0, len(_z1)):
        _z1[i], _x[i], _z2[i] = quat2euler(q[i])

#
    ------------------------------------------------------------------------------

    # Using the Rodrigues Rotation Formula, defined as R = I + sin(theta)
       * K + (1 - cos(theta))*K^2
    # with K = [0 -k_z, k_y; k_z, 0, -k_x; -k_y, k_x, 0], and the
       components of
    # k coming from the vector being rotated about.  Theta is specified by
        the misorientation.
    if useRRF:
        orientation_matrix1, orientation_matrix2 = calcRotMatRRF(axis,
           _misorientation)

        # Normalize the matrices using their determinants
        orientation_matrix1 = orientation_matrix1 / linalg.det(
           orientation_matrix1)
```

```
        orientation_matrix2 = orientation_matrix2 / linalg.det(
            orientation_matrix2)
300
        if not quiet:
302         displayMat(orientation_matrix1)
            displayMat(orientation_matrix2)
304
        for i in range(0, len(_z1)):
306         if dispEuler:
                displayAngles(_z1[i], _x[i], _z2[i])
308
            if save:
310             assert i < 2, "ERROR: Too many Euler angles."
                if i == 0:
312                 writeMat(orientation_matrix1, _z1[i], _x[i], _z2[i], '
                        P', _axis)
                else:
314                 writeMat(orientation_matrix2, _z1[i], _x[i], _z2[i], '
                        Q', _axis)
#
    ------------------------------------------------------------------------------

316  else:
        for i in range(0,len(_z1)):
318         orientation_matrix = calcRotMat(_z1[i], _x[i], _z2[i])

320         # Normalize the matrix using the determinant
            orientation_matrix = orientation_matrix / linalg.det(
                orientation_matrix)
322
            if not quiet: # Display the results
324             displayMat(orientation_matrix)
```

```
326             if dispEuler: # Display the Euler Angles
                    displayAngles(_z1[i], _x[i], _z2[i])
328
                if save: # We only calculate 2 angles at a time.  If there are
                    more, that's a problem.
330                 assert i < 2, "ERROR: Too many Euler angles."
                    if i == 0:
332                     writeMat(orientation_matrix, _z1[i], _x[i], _z2[i], 'P
                            ', _axis)
                    else:
334                     writeMat(orientation_matrix, _z1[i], _x[i], _z2[i], 'Q
                            ', _axis)
```

Appendix E

Rotation Matrix Generator

This code generates the rotation matrices used to rotate the axes to the [100] direction as required by Bulatov *et al.*'s script.

```
from __future__ import division,print_function # Automatically divides as
    floats, and considers print() a function
from sys import argv # for CLI arguments
from numpy import array,linalg # for matrix operations
from os.path import exists # For checking existence of a file
from myModules import * # For using my user-defined functions

# Helper functions
def displayHelp():
    print('''
    This script will generate the rotation matrix for the given
        misorientation axis
    Input:
        _rotation_axis      This specifies the axis around which the
            grains are
                            rotated. (type: int (100) or string ('100'))

```

```
        _gbnormal           This specifies the boundary plane normal.  (
            type:
                            int (100)  or string ('100'))
    Options:
        -s --save           Saves the resultant rotation matrix to a
            database
                            (rotation_matrix_database.m) with the
                               accompanying
                            rotation axis and misorientation type.

        -q --quiet          Suppresses output of the rotation matrix

        --help              Display this help info.
    Output:
    The output displayed will be the resultant rotation matrix for the
        given
    misorientation.
    ''')

# This function is an adaptation from MOOSE RotationMatrix class.
def rotVecToZ(vec): # Creates the rotation matrix to rotate vec to the z
    direction
    # REALLY make sure vec is normalized
    vec = vec / linalg.norm(vec)

    # Initialize our vectors
    v1 = array([[0.,0.,0.]])
    v0 = array([[0.,0.,0.]])

    # Temp vector that gives a prototype of v1 by looking at the smallest
        component of vec
    w = array([[abs(vec[0][0]), abs(vec[0][1]), abs(vec[0][2])]])
```

```
    if ( (w[0][2] >= w[0][1] and w[0][1] >= w[0][0]) or (w[0][1] >= w
        [0][2] and w[0][2] >= w[0][0]) ):
42          v1[0][0] = 1.0
    elif ( (w[0][2] >= w[0][0] and w[0][0] >= w[0][1]) or (w[0][0] >= w
        [0][2] and w[0][2] >= w[0][1]) ):
44          v1[0][1] = 1.0
    else:
46          v1[0][2] = 1.0

48      # Gram-Schmidt method to find v1
    v1 = v1 - ((v1.dot(vec.T))*vec)
50      v1 = v1 / linalg.norm(v1)

52      # v0 = v1 x vec
    v0[0][0] = v1[0][1]*vec[0][2] - v1[0][2]*vec[0][1]
54      v0[0][1] = v1[0][2]*vec[0][0] - v1[0][0]*vec[0][2]
    v0[0][2] = v1[0][0]*vec[0][1] - v1[0][1]*vec[0][0]
56
    # Rotation matrix is just:
58      rot = array([[v0[0][0], v0[0][1], v0[0][2]],
                 [v1[0][0], v1[0][1], v1[0][2]],
60               [vec[0][0],vec[0][1],vec[0][2]]])
    return rot
62
def rotVec1ToVec2(vec1, vec2):
64      rot1_to_z = rotVecToZ(vec1)
    rot2_to_z = rotVecToZ(vec2)
66      return (rot2_to_z.T).dot(rot1_to_z)

68  def writeMat(m, _axis, gbnormal): # Write the matrix and angles to a file
    tex_filename = "rotation_matrix_database.m"
70      normName = _axis + '_' + gbnormal
```

```
    var_name = "rot%snorm"%(normName)
72  if not exists(tex_filename):
        tex_file = open(tex_filename, "a")
74      tex_file.write("%Database for rotation matrices for specified
            misorientation axes\n")
        tex_file.write("
            %-------------------------------------------------------------\
            n")
76      tex_file.write("%Rotation Matrix\n")
        tex_file.write("%s=[%2.4f  %2.4f  %2.4f\n"%(var_name, m[0][0], m
            [0][1], m[0][2]))
78      tex_file.write("%2.4f  %2.4f  %2.4f\n"%(m[1][0], m[1][1], m[1][2])
            )
        tex_file.write("%2.4f  %2.4f  %2.4f];\n"%(m[2][0], m[2][1], m
            [2][2]))
80      tex_file.write("
            %-------------------------------------------------------------\
            n")
        tex_file.close()
82  else:
        # Check for already written
84      numlines = countFileLines(tex_filename)
        if numlines <= 4:
86          tex_file = open(tex_filename, "a")
            tex_file.write("%s=[%2.4f  %2.4f  %2.4f\n"%(var_name, m[0][0],
                m[0][1], m[0][2]))
88          tex_file.write("%2.4f  %2.4f  %2.4f\n"%(m[1][0], m[1][1], m
                [1][2]))
            tex_file.write("%2.4f  %2.4f  %2.4f];\n"%(m[2][0], m[2][1], m
                [2][2]))
90          tex_file.write("
                %-------------------------------------------------------------\
```

```
                n")
            tex_file.close()
92      else:
            f = open(tex_filename,"r")
94          while True:
                data = f.readline().split()
96              if not data:
                    break
98              elif len(data[0]) > 14:
                    if not data[0][14] == '=':
100                     continue
                    else:
102                     if data[0][0:10] == var_name:
                            unique = False
104                     else:
                            unique = True
106         if unique:
                tex_file = open(tex_filename, "a")
108             tex_file.write("%s=[%2.4f  %2.4f  %2.4f\n"%(var_name, m
                    [0][0], m[0][1], m[0][2]))
                tex_file.write("%2.4f  %2.4f  %2.4f\n"%(m[1][0], m[1][1],
                    m[1][2]))
110             tex_file.write("%2.4f  %2.4f  %2.4f];\n"%(m[2][0], m
                    [2][1], m[2][2]))
                tex_file.write("
                    %-----------------------------------------------------------------\
                    n")
112             tex_file.close()

114 # Check what we were given...
    if "--help" in argv: # Help info
116     displayHelp()
```

```
        exit()
118
    save, argv = check4Save(argv)
120 quiet, argv = check4Quiet(argv) # Checks for suppressing output

122 if len(argv) != 3: # if not both values given
        print("ERROR: Incorrect number of command line arguments. Line 150")
124     displayHelp()
        exit()
126 else: # len(argv) == 3
        script, _rotation_axis, _gbnormal = argv
128
    if not type(_gbnormal) in {int, str}:
130     print("ERROR: Grain boundary normal type is incorrect.  Please enter
            an int or a string. Line 157")
        print("You entered %s with type %s"%(str(_gbnormal), type(_gbnormal)))
132     exit()
    else:
134     if type(_gbnormal) == int:
            _gbnormal = '0' + '0' + '0' + str(_gbnormal)
136         _gbnormal =_gbnormal[-3:] # gets the last three characters
            assert _gbnormal != '000', "ERROR: invalid boundary normal. Line
                173"
138
        assert(len(_rotation_axis) == 3), "ERROR: Something went wrong
            converting _gbnormal into a string. Line 166"
140
    if not type(_rotation_axis) in {int, str}:
142     print("ERROR: Grain boundary rotation axis type is incorrect.  Please
            enter an int or a string. Line 169")
        print("You entered %s with type %s"%(str(_rotation_axis), type(
            _rotation_axis)))
```

```
144     exit()
else: # Convert anything besides a string into a string
146     if type(_rotation_axis) == int:
            _rotation_axis = '0' + '0' + '0' + str(_rotation_axis)
148         _rotation_axis = _rotation_axis[-3:] # Get the last three
                characters
            assert _rotation_axis != '000', "ERROR: invalid rotation axis.
                Line 176"
150
        assert(len(_rotation_axis) == 3), "ERROR: Something went wrong
            converting _rotation_axis into a string. Line 178"
152
# Now that the input is taken care of, do the work
154 axis = array([[1, 0, 0]]) # This is the axis that we rotate the grain
        boundary normal to

156 # This part converts _gbnormal to an array for use in the rotation
        functions
gbnormal = array([[None]*3])
158 j = 0
indices = []
160 for i in range(0,len(gbnormal[0])):
        try:
162         gbnormal[0][i] = int(_gbnormal[j])
            j = j+1
164     except:
            #print(_gbnormal[i:i+2])
166         gbnormal[0][i] = int(_gbnormal[j:j + 2])
            j = j + 2
168         indices.append(i)

170
```

```
    # So much work...
172 gbnorm = ''
    for i in range(0,len(gbnormal[0])):
174     if gbnormal[0][i] < 0:
            gbnorm += str(abs(gbnormal[0][i])) + 'bar'
176     else:
            gbnorm += str(gbnormal[0][i])
178 gbnormal = gbnormal / linalg.norm(gbnormal) # Normalize the gbnormal
       vector.
    axis = axis / linalg.norm(axis) # Just to be sure...
180 rotation_matrix = rotVec1ToVec2(gbnormal, axis)


182


184 if not quiet:
        displayMat(rotation_matrix)
186 if save:
        writeMat(rotation_matrix, _rotation_axis, gbnorm)
```

Appendix F

genOrientationMatrix.sh Bash Script

This bash script reads a CSV file containing misorientation angles data, and uses those angles to generate the P and Q matrices. This script calls the script `orientation_matrix.py`.

```
#! /bin/bash

# This script will generate the orientation matrices through python by
    looping
# through the CSV values given in the input files.
# Argument(s):
#    $1       Should be a filename that specifies the angles and relative
#             energies for the 100, 110, and 111 symmetric tilt and twist
#             boundaries

# Command-line argument counter that checks for the correct number of
    arguments.
# Does not check for correct syntax.
if [ "$#" -ne 1 ]; then
  echo "Illegal number of parameters"
  exit 1
fi

```

```
# This takes the first argument from the command line - this is assumed to be a
# filename of the format 100Tilt.
FN=$1

echo "Determining the axis..."
# Pulls out the axis from the input file name.  This uses regex syntax to find
# a series of numbers that match either 100, 110, or 111.  This also has an issue
# where it will find a match for 101, but as long as the files are named correctly
# it shouldn't be an issue.
AXIS=`echo $FN | grep -o "1[01][01]"`

echo "Reading the file..."
IFS="," # separation character is the comma
# Exit with error code 99 if unable to read the file
[ ! -f $FN ] && { echo "$FN file not found"; exit 99; }

# This makes the assumption that the file orientation_matrix.py has executable
# rights.
echo "Running the command: ~/projects/scripts/orientation_matrix.py $AXIS <angle> -s -q"
while read -r angle en; do # read the file with comma separated values

  ~/projects/scripts/orientation_matrix.py $AXIS $angle -s -q
done < "$FN" # the "$FN" is required if it's going to run properly!

IFS=$OLDIFS # go back to the old separation character based on the system value.
```