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	⟨100⟩ Max Distance	0.405
3	⟨110⟩ Max Distance	0.739
4	⟨111⟩ Max Distance	0.352
5	⟨100⟩ Weight	50.5
6	⟨110⟩ Weight	4.55
7	⟨111⟩ Weight	0.08
8	⟨100⟩ Tilt/Twist Mix Power Law (1)	0.03325
9	⟨100⟩ Tilt/Twist Mix Power Law (2)	0.00053125
10	Maximum ⟨100⟩ Twist Energy	0.60903
11	⟨100⟩ Twist Shape Factor	1.4486
12	⟨100⟩ Asymmetric Tilt Interpolation Power	35.8
13	⟨100⟩ Symmetric Tilt First Peak Energy	1.0058
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

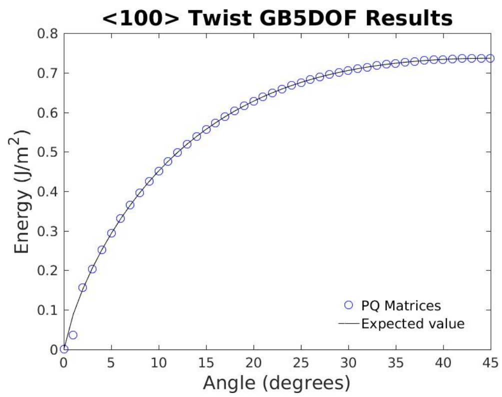
Continued on next page.

Table A.1 – *Continued from previous page*

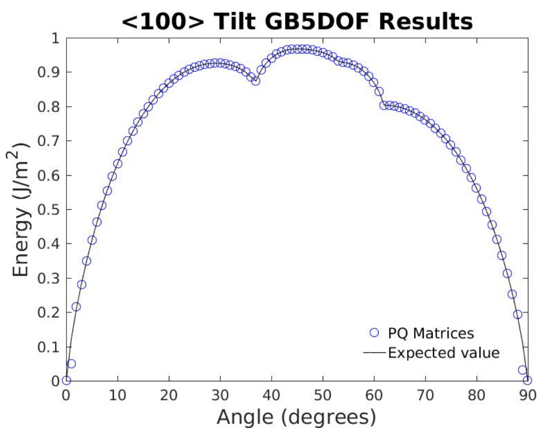
Array number	Parameter name	Parameter value
20	$\langle 110 \rangle$ Tilt/Twist Mix Power Law (1)	3.1573
21	$\langle 110 \rangle$ Tilt/Twist Mix Power Law (2)	1.9784
22	$\langle 110 \rangle$ Twist Peak Angle	0.46145
23	$\langle 110 \rangle$ Twist Peak Energy	1.1444
24	$\langle 110 \rangle$ Twist $\Sigma 3$ Energy	1.0931
25	$\langle 110 \rangle$ Twist 90° Energy	1.152
26	$\langle 110 \rangle$ Asymmetric Tilt Shape Factor	3.1843
27	$\langle 110 \rangle$ Symmetric Tilt Third Peak Energy	1.0514
28	$\langle 110 \rangle$ Symmetric Tilt $\Sigma 3$ Energy	0.61703
29	$\langle 110 \rangle$ Symmetric Tilt Second Peak Energy	1.0902
30	$\langle 110 \rangle$ Symmetric Tilt $\Sigma 11$ Energy	0.56686
31	$\langle 110 \rangle$ Symmetric Tilt First Peak Energy	1.1024
32	$\langle 110 \rangle$ Symmetric Tilt Third Peak Angle	0.88736
33	$\langle 110 \rangle$ Symmetric Tilt Second Peak Angle	1.8711
34	$\langle 110 \rangle$ Symmetric Tilt First Peak Angle	2.731
35	$\langle 111 \rangle$ Tilt-Twist Linear Interpolation	38.201
36	$\langle 111 \rangle$ Twist Shape Factor	1.2414
37	$\langle 111 \rangle$ Twist Peak Angle	0.49979
38	$\langle 111 \rangle$ Twist Peak Energy	0.7971
39	$\langle 111 \rangle$ Symmetric Tilt Peak Angle	0.25966
40	$\langle 111 \rangle$ Symmetric Tilt Max Energy	1.0288
41	$\langle 111 \rangle$ Symmetric Tilt $\Sigma 3$ Energy	1.1311
42	$\langle 111 \rangle$ Asymmetric Tilt Symmetry Point Energy	3.7674
43	$\langle 111 \rangle$ Asymmetric Tilt Scale Factor	0.053417

Appendix B

Graphs

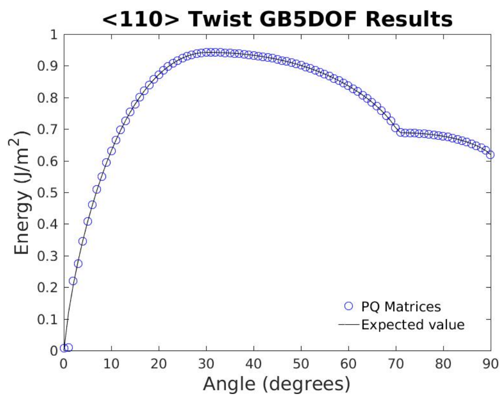


(a)

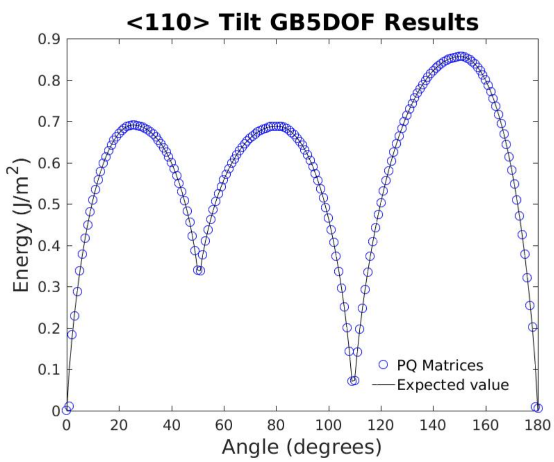


(b)

Figure B.1: The $\langle 100 \rangle$ 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.

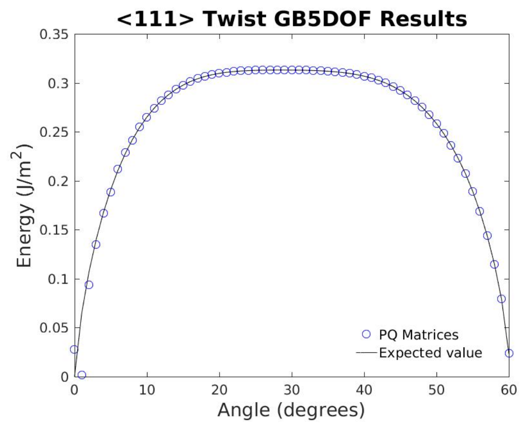


(a)

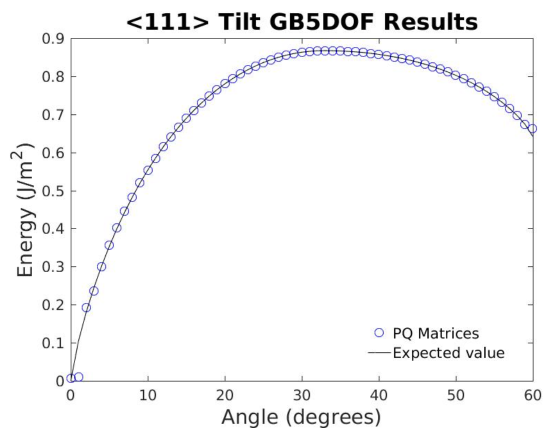


(b)

Figure B.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.

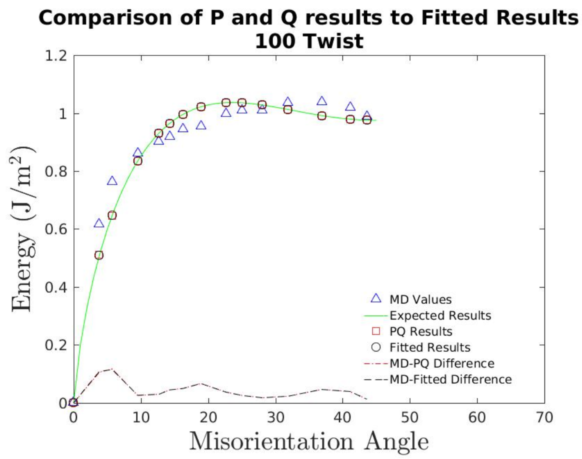


(a)

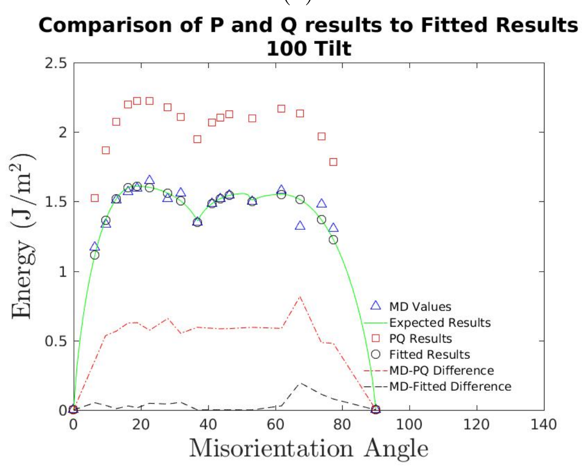


(b)

Figure B.3: The $\langle 111 \rangle$ 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.

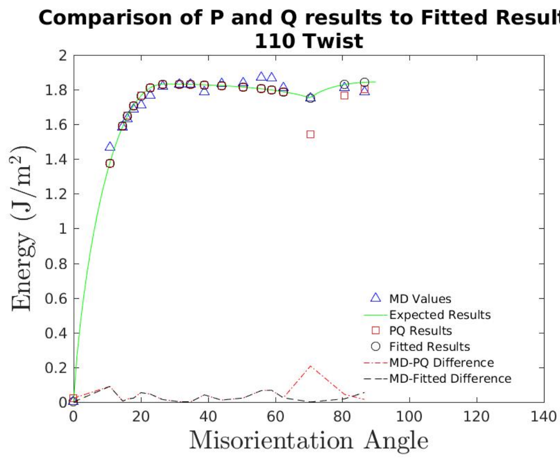


(a)

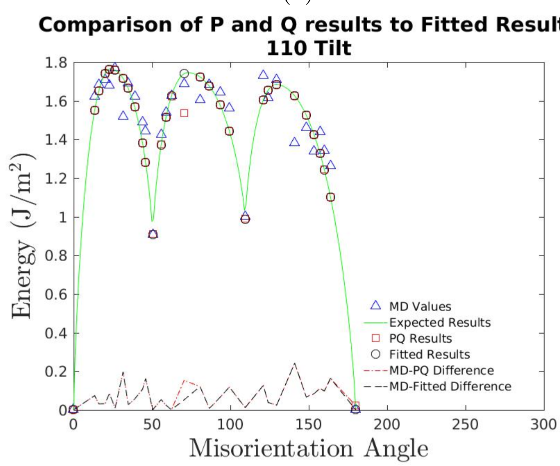


(b)

Figure B.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 is causing the scaling issue for this subset.

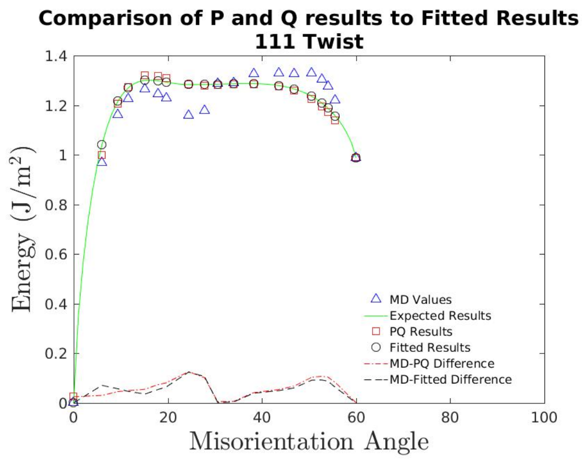


(a)

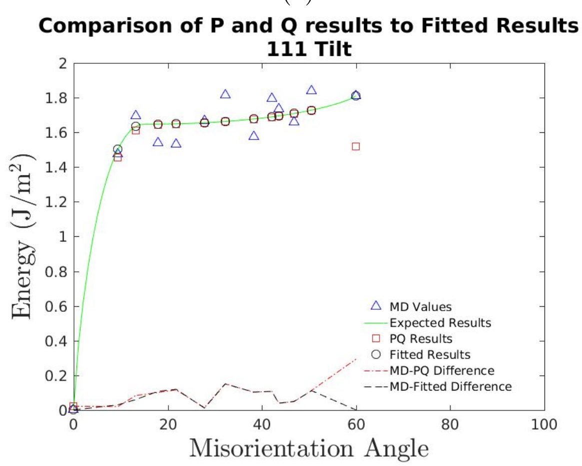


(b)

Figure B.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.



(a)



(b)

Figure B.6: A comparison of the expected value of the fitted function with the values calculated using the P and Q matrices for the $\langle 111 \rangle$ 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 C

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.

```
#! /usr/bin/env python

# 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)
#   _misorientation: The angle of misorientation (type:
    float)
#             ----------OR----------
#    (with option -e or --euler)
#   _z1: The first rotation angle  (Z ) (type: float)
#   _x:  The second rotation angle (X') (type: float)
#   _z2: The third rotation angle  (Z") (type: float)
#
# If the option -e or --euler-angles is entered, the
    calculation skips to simply
# output the orientation matrices.  Otherwise, the
    Euler angles are calculated from
# the axis, orientation, and grain boundary normal, and
    then the orientation matrix is
```

```
# created through the use of the Rodrigues Rotation
    Formula, which is:
# R = I + sin(theta) * K + (1 - cos(theta))*K^2
# where I is the identity matrix, theta is the
    misorientation angle, and K is
# the skew-symmetric matrix formed by the axis of
    rotation:
# K = 0  -kz   ky
#      kz   0  -kx
#    -ky   kx   0
# where the vector k is the unit vector defining the
    axis of rotation, or using
# 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
# to.  If the user does not specify to save, then the
    angles are not used for
# anything.
#
# Options:
# -e --euler <_z1> <_x> <_z2>              Returns the
    Bunge orientation matrix
#                                          based on the
    euler angles provided.
#
# -f --file <filename>                     Reads the file
    filename and uses the
#                                          Euler angles
    from them to calculate the
#                                          orientation
    matrix.
#
# --rrf                                    Calculates the
    matrices using the Rodrigues
#                                          Rotation
    Formula
#
```

```
# -a --angles                                    Displays the
   Euler angles.  Can be used
#                                                in conjunction
   with -q or --quiet to
#                                                display only
   the Euler angles.
#
# -s --save                                      Saves the
   resultant orientation matrix to
#                                                a database (
   orientation_matrix_database.m)
#                                                with the
   accompanying Euler angles.
#
# -q --quiet                                     Suppresses
   output of the orientation matrices
#                                                to the terminal
#
# --help                                         Displays this
   help info
#
# Output:
# For an Euler angle set, the ouput is simply its
   orientation matrix.
# For the misorientations, the first matrix is the 'P'
   orientation matrix, and
# the second matrix is the 'Q' orientation matrix (see
   Bulatov et al., Acta Mater
# 65 (2014) 161-175).

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)
        _misorientation: The angle of misorientation (
           type: float)
           ----------OR----------
        (with option -e or --euler)
        _z1: The first rotation angle  (Z ) (type:
           float)
        _x:  The second rotation angle (X') (type:
           float)
        _z2: The third rotation angle  (Z") (type:
           float)

    If the option -e or --euler-angles is entered, the
       calculation skips to simply
    output the orientation matrices.  Otherwise, the
       Euler angles are calculated from
    the axis, orientation, and grain boundary normal,
       and then the orientation matrix is
    created through the use of the Rodrigues Rotation
       Formula, which is:
    R = I + sin(theta) * K + (1 - cos(theta))*K^2
    where I is the identity matrix, theta is the
       misorientation angle, and K is
    the skew-symmetric matrix formed by the axis of
       rotation:
    K = 0  -kz   ky
```

```
   kz   0  -kx
  -ky   kx   0
where the vector k is the unit vector defining the
   axis of rotation, or using
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
to.  If the user does not specify to save, then the
    angles are not used for
anything.

Options:
-e --euler <_z1> <_x> <_z2>              Returns the
   Bunge orientation matrix
                                         based on the
                                            euler angles
                                             provided.

-f --file <filename>                     Reads the file
   filename and uses the
                                         Euler angles
                                            from them to
                                             calculate
                                            the
                                         orientation
                                            matrix.

--rrf                                    Calculates the
   matrices using the Rodrigues
                                         Rotation
                                            Formula

-a --angles                              Displays the
   Euler angles.  Can be used
                                         in conjunction
                                            with -q or
                                           --quiet to
```

```
                                                display only
                                                   the Euler
                                                   angles.

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

    -q --quiet                                  Suppresses
       output of the orientation matrices
                                                to the terminal

    --help                                      Displays this
       help info

    Output:
    For an Euler angle set, the ouput is simply its
       orientation matrix.
    For the misorientations, the first matrix is the 'P
       ' orientation matrix, and
    the second matrix is the 'Q' orientation matrix (
       see Bulatov et al., Acta Mater
    65 (2014) 161-175).
    ''')
    return

def displayAngles(z1, x, z2): # Displays an Euler angle
    set (Bunge convention)
    print("Euler angles:")
    # This is the "new" way to format strings.  The 16
       indicates the padding to
```

```
    # be done before the next character.  The '<'
        character below says which side
    # to pad (the right side).
    print("{:16}{:16}{:16}".format('Z', 'X', 'Z'))
    print("------------------------------------------------")
    print("{:<16}{:<16}{:<16}\n".format(rad2deg(z1),
        rad2deg(x), rad2deg(z2)))
    return

def check4RRF(args): # Check the args for the rrf
    command
    if "--rrf" in args:
        index = args.index("--rrf")
        del args[index]
        return True, args
    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")
    tex_file.write("
       %
       n")
    tex_file.write("%Orientation Matrix             
                                Euler Angles\n")
    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]))
    tex_file.write("%2.6f  %2.6f  %2.6f];\n"%(m
       [2][0], m[2][1], m[2][2]))
    tex_file.write("
       %
       n")
    tex_file.close()
else:
    f = open(tex_filename,"r")
    while True:
        data = f.readline().split()
        if not data:
            break
        elif len(data) != 6:
            continue
```

```
else:
    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]:
        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()
```

```python
                # 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
        if unique:
            tex_file = open(tex_filename, "a")
            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]))
            tex_file.write("%2.6f  %2.6f  %2.6f];\n"%(m
               [2][0], m[2][1], m[2][2]))
            tex_file.write("
               %-------------------------------------------------------------------------------
               n")
            tex_file.close()
    return

if "--help" in argv: # Help info
    displayHelp()
    exit()

orientation_matrix = []
save, argv = check4Save(argv) # Save the file?  Delete
   the save argument
quiet, argv = check4Quiet(argv) # Checks for
   suppressing output. Delete the quiet argument.
```

```
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

# If the arguments come from a file...
if "-f" in argv or "--file" in argv: #input arguments come from file
    try:
        try:
            index = argv.index("-f")
        except:
            index = argv.index("--file")
    except:
        print("ERROR: Unable to find filename.")
        exit()
    filename = argv[index + 1]
    try:
        f1 = open(filename, 'r')
    except:
        print("ERROR: Unable to read file.", filename)

    while True: # Read the file line by line.
        line = f1.readline()
        # break if we don't read anything.  If there are blank lines in the
        # file, this will evaluate to TRUE!
        if not line:
            break;
        data = line.split()
        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
        else:
            # Convert the data to stuff we can use
            _z1 = float(data[0])
```

```
            _x  = float(data[1])
            _z2 = float(data[2])

            _z1 = deg2rad(_z1)
            _x  = deg2rad(_x)
            _z2 = deg2rad(_z2)
            orientation_matrix = calcRotMat(_z1, _x,
                _z2)
            if not quiet:
                displayMat(orientation_matrix)
            if save:
                writeMat(orientation_matrix, _z1, _x,
                    _z2,'P', _axis)

# Input is a set of euler angles
elif "-e" in argv or "--euler-angles" in argv:
    try:
        try:
            index = argv.index("-e")
        except:
            index = argv.index("--euler-angles")
    except:
        print("ERROR: Unable to read Euler angles.")
        exit()
    _z1 = float(argv[index + 1])
    _x =  float(argv[index + 2])
    _z2 = float(argv[index + 3])
    _z1 = deg2rad(_z1)
    _x  = deg2rad(_x)
    _z2 = deg2rad(_z2)

    orientation_matrix = calcRotMat(_z1, _x, _z2)

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

```
else:
    if len(argv) < 3:
        print("ERROR: Not enough command line arguments
            .")
        print("Input either an axis, and a
            misorientation, or a ZXZ Euler angle set
            with the option -e or --euler-angles.")
        displayHelp()
        exit()
    try:
        _axis = int(argv[1])
        _misorientation = float(argv[2])
    except:
        print('''
        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()

    if not len(str(_axis)) == 3: # axis length greater
        than 3
        print("ERROR: Argument 1 must by a 3 digit
            number like \'100\'.")
        exit()

    _misorientation = deg2rad(_misorientation) # Change
        input to radians
    axis = [None]*3
    _z1 = [None]*2
    _x = [None]*2
    _z2 = [None]*2
    q = [None]*2
    for i in range(0, len(str(_axis))):
        axis[i] = int(str(_axis)[i])
```

```
#
    ----------------------------------------------------------------------
#----------------------------------------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)

        if not quiet:
            displayMat(orientation_matrix1)
            displayMat(orientation_matrix2)

        for i in range(0, len(_z1)):
            if dispEuler:
                displayAngles(_z1[i], _x[i], _z2[i])
```

```
            if save:
                assert i < 2, "ERROR: Too many Euler angles."
                if i == 0:
                    writeMat(orientation_matrix1, _z1[i], _x[i], _z2[i], 'P', _axis)
                else:
                    writeMat(orientation_matrix2, _z1[i], _x[i], _z2[i], 'Q', _axis)
#
```

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

            if not quiet: # Display the results
                displayMat(orientation_matrix)

            if dispEuler: # Display the Euler Angles
                displayAngles(_z1[i], _x[i], _z2[i])

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

Appendix D

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.
```