Homework 7: Misorientations
A.D. Rollett, 27-750, Texture, Microstructure and Anisotropy

Due date: 26th March, 2016

Q1. [10 points]
Starting with a set of Miller indices (3 1 -1) [1 0 3], compute the equivalent i) Euler angles in degrees, ii) unit quaternion, iii) angle and axis, iv) Rodrigues-Frank vector and v) orientation matrix

Q2. [50 points]
(a) You are given a list of orientations and your task is to calculate the misorientations between them. Apply the algorithm that applies crystal symmetry to both sides of the misorientation and chooses the smallest possible magnitude of misorientation i.e. smallest rotation angle. Also select the result that places the misorientation axis in the same unit triangle as the list of CSLs that use in part b) below. If you use the list provided in the lecture notes, that means {h>=0, k>=0, l>=0, h>=k>, k>=l}. You may use any method that is convenient to you. Matrices are acceptable, unit quaternions will teach you something new and Rodrigues vectors are inadvisable (because any 180° operator results in infinities). Remember also to include switching symmetry in addition to the crystal symmetry operators. You must calculate both the magnitude of the **misorientation** and the **rotation axis**. Also give the values of the Rodrigues vectors that correspond to each axis-angle set.
(b) Also compute how near each misorientation is to each CSL type up to Σ=29 and record how near it is in terms of the Brandon criterion. Remember that the angle that you quote for the "nearness" must be the **minimum misorientation angle**, which is what we generally take as the physically most meaningful quantity. Remember that it is important to have the misorientation axis (that is associated with the minimum angle misorientation) in the same unit triangle as the CSL. Finally, each of these texture components has 1, 2 or 4 variants, based on the orthorhombic sample symmetry. You must calculate the misorientations between each possible pair of component+variant because each variant is a physically distinct orientation related via *sample symmetry* (try sketching pole figures for the variants to convince yourself about this, if it is not immediately obvious). This means that you will have to generate the set of Euler angles (or whichever representation that you use) for the variants before you compute the misorientations. Recall that you computed equivalent descriptions of orientations when you worked with pole figures including both crystal and sample symmetry. You must include a copy of your Matlab code with your submission to show how you performed the calculation.

No.	Name	Indices	Bunge (φ_1,Φ,φ_2) RD= 1	Number of Variants (sample symmetry)
1	Copper	{112}⟨11$\bar{1}$⟩	90.0, 35.2644, 45.0	2
2	S3	{213}⟨3 6$\bar{4}$⟩	59, 37, 63	4
3	Brass	{110}<112>	35.2644, 45.0, 0.0	2

To aid you in confirming that your calculations are coming out correctly, the table below lists the misorientation angles (to two significant figures) that can arise between each combination of components.

	Copper	**S3**	**Brass**
Copper	0, 60°	19°, 51°	36°
S3		[you tell me!]	19°, 54°
Brass			0°, 60°

Your final submission should look like this. Note that each entry has only one angle and axis, so be sure to sort your answers properly. If the misorientation angle is zero (i.e. no grain boundary) then the axis is irrelevant, obviously, and no entry is needed. Note that a number of the entries are repeats of each other. Because of switching symmetry, only the upper right triangle (or lower left) need be filled in.

Table of Misorientation Angles and Axes

	Euler angles	**Copper, 1st**	**Copper, 2nd**	**Brass, 1st**	**Brass, 2nd**	**S3, 1st**	**S3, 2nd**	**S3, 3rd**	**S3, 4th**
Copper, 1st variant		0	60°, <111> {1/3,1/3,1						

			/3}						
Copper, 2nd variant			0						
Brass, 1st variant				0					
Brass, 2nd variant					0				
S3, 1st variant						0			
S3, 2nd variant							0		
S3, 3rd variant								0	
S3, 4th variant									0

Q3. [15 points] The maximum misorientation angle that is possible between two cubic crystals has been given (in L12). (a) Explain how the value is obtained (hint: refer to Rodrigues space) in relation to crystal symmetry elements. (b) Now repeat the calculation for hexagonal crystals and determine the maximum possible misorientation between, e.g., a pair of zirconium crystals.

Q4. [10 points] The shape of the FZ for orientations of hexagonal materials is a 12-sided prism, see the diagram 1.5(d) reproduced from the book by Sutton & Balluffi below. Explain in detail which symmetry operator produces each facet on the prism and how to obtain the dimensions indicated.

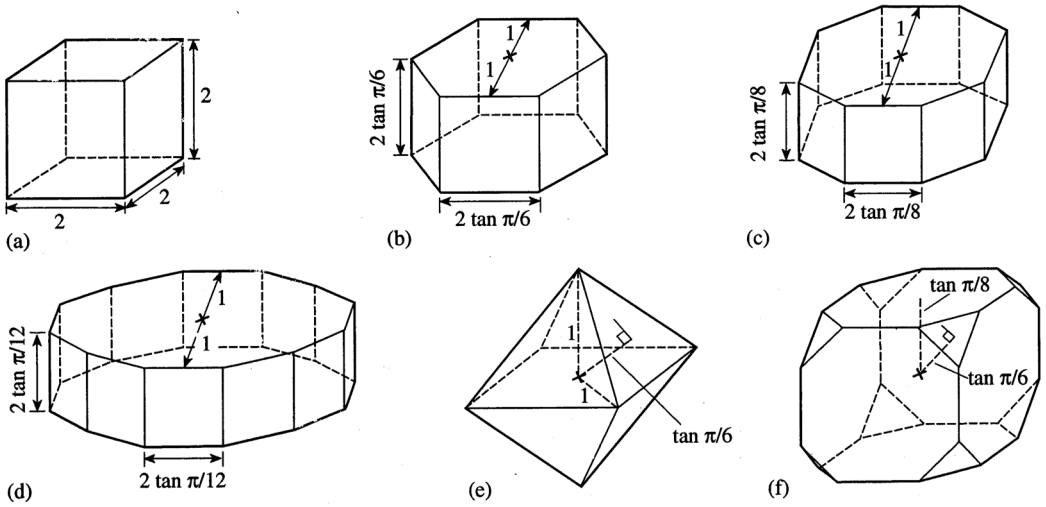

Fig. 1.5 The fundamental zones of the forms of closed polyhedra: (a) cube for the point groups 222, 2*mm*, *mmm* of the orthorhombic system; (b) hexagonal prism for 32, $\bar{3}m$, 3*m* of the trigonal system; (c) octagonal prism for 422, 4/*mmm*, 4*mm*, and $\bar{4}2m$ of the tetragonal system; (d) dodecagonal prism for 622, 6/*mmm*, 6*mm*, and $\bar{6}m2$ of the hexagonal system; (e) octahedron for 23 and $m\bar{3}$ of the cubic system; (f) semiregular truncated cube for 432, $m\bar{3}m$, and $\bar{4}3m$ of the cubic system.

Q5. [15 points]

Make sketches of the Σ9, Σ19a, and Σ11 CSL relationships. Use the construction discussed in the class with two overlapped grids; the grid shown below may be helpful (but think about why it is not square). Label the axes of the grid with the crystallographic directions. Write out the Rodrigues vectors as integer fractions (Hint: the answers are available in the lecture notes but you must show how to obtain the result). Also give the angle in degrees for each of the CSL types. It may help to draw out the Coincident Site Lattice for, say, the Σ9 case and identify the coincident versus the non-coincident points for one of the lattices.