Homework 4: Calculation of Misorientations

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Q1.
Description: you are given a list of orientations and your task is to calculate the misorientations between them, being careful to find the smallest misorientation possible. You may use any method that is convenient to you. 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. 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 must be the **minimum misorientation angle**, which is what we generally take as the physically most meaningful quantity. To make the latter easier, you may use the axis that is associated with the minimum misorientation matrix even though it may have some negative values [sorting out which symmetry operators place the all the axes in the same stereographic triangle is harder to do]. Remember also to include switching symmetry in addition to the crystal symmetry operators. Finally, each of these components has several variant positions, 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 (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 [suggestion: you can use *mill2eul.f* to compute all the equivalent Euler angles for a specific texture component].

No.	**Name**	**Indices**	**Bunge (φ_1,Φ,φ_2) RD= 1**	**Number of Variants (sample symmetry)**
1	copper	$\{112\}\langle 11\bar{1}\rangle$	40, 65, 26	2
2	S3	$\{213\}\langle 3\,6\,4\rangle$	59, 37, 63	4
3	Brass	{110}<112>	35, 45, 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 there is no misorientation (no grain boundary!) then the axis is irrelevant, obviously.

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							0		

variant									
S3, 3rd variant								0	
S3, 4th variant									0