

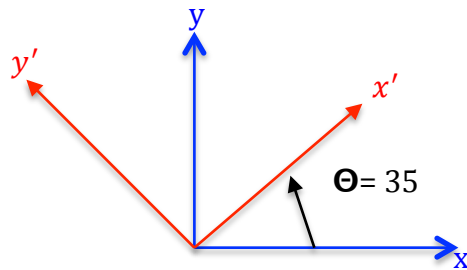
Homework 2; **different representations of orientations (as rotations), effect of crystal and sample symmetry.** Solution Set as of 23rd Jan '16

Due: 11:59pm, Weds, Jan. 27th.

You are expected to do the numerical exercises in Matlab. For each answer, provide your Matlab script along with the values and/or graphs. As usual, there is no problem about working together but you have to provide individual answers (i.e. there had better not be any identical Matlab scripts!).

1. [35] In this exercise, we learn how to apply an axis transformation.

- Draw a pair of orthogonal x-y axes (hint: the arrow.m package for Matlab is helpful, which is posted on blackboard), with x pointing to the right, and y up the page (i.e. the standard arrangement);
- Draw a second pair of x'-y' axes that are rotated with respect to the first pair by 35° (hint: a positive angle corresponds to an anti-clockwise rotation, looking down the rotation axis, which is equivalent to the right-hand rule);



c. Calculate the coefficients of the transformation matrix;

$$a_{ij} = \begin{bmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 0.82 & 0.57 & 0 \\ -0.57 & 0.82 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

d. Compute the coefficients of the unit vector parallel to [410] in the first frame, assuming that x and y are parallel to [100] and [010], respectively;

$$v_i = [410], |v| = \sqrt{4 * 4 + 1 * 1 + 0} = \sqrt{18} = 4.243$$

$$\hat{v}_1 = \frac{4}{4.243} = 0.943$$

$$\hat{v}_2 = \frac{1}{4.243} = 0.236$$

$$\hat{v}_3 = \frac{0}{4.243} = 0$$

e. Compute the coefficients of this same vector in the new, primed frame;

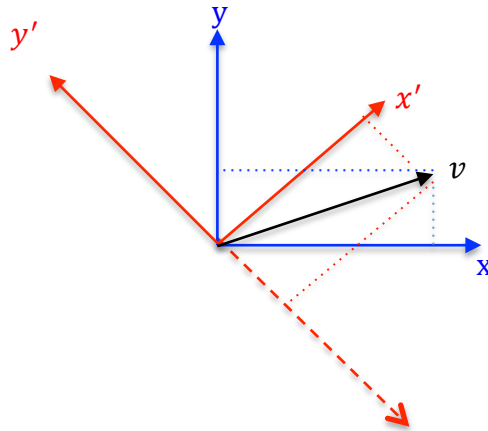
$$\dot{v}_i = a_{ij}v_j$$

$$\dot{v}_1 = a_{11}v_1 + a_{12}v_2 + a_{13}v_3 = 0.82*0.943 + 0.57*0.236 + 0*0 = 0.91$$

$$\dot{v}_2 = a_{21}v_1 + a_{22}v_2 + a_{23}v_3 = -0.57*0.943 + 0.82*0.236 + 0*0 = -0.344$$

$$\dot{v}_3 = a_{31}v_1 + a_{32}v_2 + a_{33}v_3 = 0*0.943 + 0*0.236 + 0*1 = 0$$

f. Draw the vector in the same diagram;



g. A stress tensor cannot be drawn as easily as a vector. Therefore this part asks you to compute the coefficients in the new frame from the following stress tensor.

$$\sigma_{ij} = \begin{bmatrix} 10 * \sqrt{2} & 5 * \sqrt{2} \\ 5 * \sqrt{2} & 15 * \sqrt{2} \end{bmatrix}$$

$$\dot{\sigma}_{ij} = a_{ik}a_{jl}\sigma_{kl}$$

$$\begin{aligned} \dot{\sigma}_{11} &= a_{1k}a_{1l}\sigma_{kl} = a_{11}a_{11}\sigma_{11} + a_{11}a_{12}\sigma_{12} + a_{12}a_{11}\sigma_{21} + a_{12}a_{12}\sigma_{22} = \\ & (0.82*0.82*10*\sqrt{2}) + (0.82*0.57*5*\sqrt{2}) + (0.57*0.82*5*\sqrt{2}) + (0.57*0.57*15*\sqrt{2}) = 23.01 \end{aligned}$$

$$\begin{aligned} \dot{\sigma}_{12} &= a_{1k}a_{2l}\sigma_{kl} = a_{11}a_{21}\sigma_{11} + a_{11}a_{22}\sigma_{12} + a_{12}a_{21}\sigma_{21} + a_{12}a_{22}\sigma_{22} = (0.82* \\ & -0.57*10*\sqrt{2}) + (0.82*0.82*5*\sqrt{2}) + (0.57*-0.57*5*\sqrt{2}) + (0.57*0.82*15*\sqrt{2}) = 5.76 \end{aligned}$$

$$\begin{aligned} \sigma_{21} &= a_{2k}a_{1l}\sigma_{kl} = a_{21}a_{11}\sigma_{11} + a_{21}a_{12}\sigma_{12} + a_{22}a_{11}\sigma_{21} + a_{22}a_{12}\sigma_{22} = \\ &(-0.57*0.82*10*\sqrt{2})+(-0.57*0.57*5*\sqrt{2})+(0.82*0.82*5*\sqrt{2})+(0.82*0.57*15*\sqrt{2})= \\ &5.76 \end{aligned}$$

$$\begin{aligned} \sigma_{22} &= a_{2k}a_{2l}\sigma_{ll} = a_{21}a_{21}\sigma_{11} + a_{21}a_{22}\sigma_{12} + a_{22}a_{21}\sigma_{21} + a_{22}a_{22}\sigma_{22} = (-0.57*- \\ &0.57*10*\sqrt{2})+(-0.57*0.82*5*\sqrt{2})+(0.82*-0.57*5*\sqrt{2})+(0.82*0.82*15*\sqrt{2})=12.248 \end{aligned}$$

$$\sigma_{ij} = \begin{bmatrix} 23.01 & 5.76 \\ 5.76 & 12.248 \end{bmatrix}$$

Matlab Hint: in a matlab script, the commands “w2 = figure(1);” and “print(w2, '-dpng', fileOut);”, where fileOut is the filename of the graph to be saved, and the plotting commands are between these two lines, are helpful.

Another Matlab hint: this set of lines can be helpful for saving plots in your current directory.

```
“path = mfilename('fullpath');
[folder, name, ext] = fileparts(path);
fprintf(' current directory = %s \n',folder);
fileName = input('Enter a name for the Output file (.png will be added): ','s');
fileOut = strcat(folder,'/',fileName,'.png');”
```

2. [20] In this exercise, we see how to perform a vector (active) rotation.

- Draw the same x-y frame;
- Draw the same unit vector parallel to [410] as above;
- Write out the transpose of the transformation matrix that you obtained above, which is the matrix that represents the corresponding rotation.

$$b_{ij} = a_{ij}^T = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} = \begin{bmatrix} 0.82 & -0.57 \\ 0.57 & 0.82 \end{bmatrix}$$

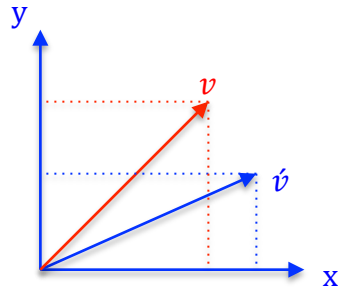
d. Compute and draw the new rotated vector.

$$\hat{v}_i = b_{ij}v_j$$

$$\hat{v}_1 = b_{11}v_1 + b_{12}v_2 + b_{13}v_3 = 0.82*0.943+ -0.57*0.236+ 0*0= 0.639$$

$$\hat{v}_2 = b_{21}v_1 + b_{22}v_2 + b_{23}v_3 = 0.57*0.943+ 0.82*0.236+ 0*0= 0.731$$

$$\hat{v}_3 = b_{31}v_1 + b_{32}v_2 + b_{33}v_3 = 0*0.943+ 0*0.236+ 0*1=0$$



3. [30 points]

The exact location of the "S" texture component in Euler space is somewhat debated in the literature, so we will (somewhat arbitrarily) assign it values of (32°, 58°, 18°).

a. Convert the Euler angles to a matrix.

Here we can use SteveSintay_Pole_Figures etc., although the `variants_ADR.m` script also provides it.

Rotation Matrix, g (Passive Axis transformation)		
0.719765238	0.642854487	0.262061274
-0.529131664	0.263647909	0.806541668
0.449397023	-0.719185573	0.529919264

b. Apply crystal symmetry and generate the 24 equivalent points. Convert each result from a matrix to Euler angles and list the result. Try to make as compact a table of values as you can (i.e. include 4 columns with the 1st being the number of the symmetry operator and the other 3 columns containing the 3 Euler angles).

Used `variants_ADR.m` (in Matlab)

loop_number	phi1	PHI	phi2	(degrees)
1	32.0000	58.0000	18.0000	18.0000
2	212.0000	122.0000	162.0000	162.0000
3	243.5145	36.2406	153.6862	153.6862
4	63.5145	143.7594	26.3138	26.3138
5	212.0000	122.0000	342.0000	342.0000
6	32.0000	58.0000	198.0000	198.0000
7	63.5145	143.7594	206.3138	206.3138
8	243.5145	36.2406	333.6862	333.6862
9	32.0000	58.0000	108.0000	108.0000
10	311.7695	105.1924	123.3060	123.3060
11	212.0000	122.0000	72.0000	72.0000

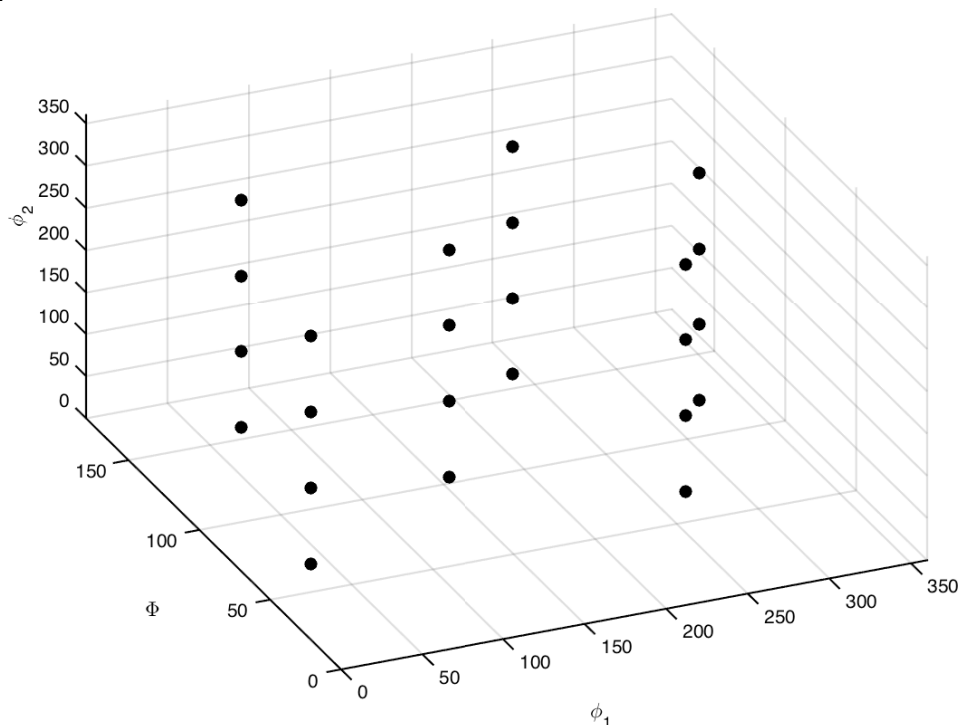
12	131.7695	74.8076	56.6940
13	32.0000	58.0000	288.0000
14	131.7695	74.8076	236.6940
15	212.0000	122.0000	252.0000
16	311.7695	105.1924	303.3060
17	311.7695	105.1924	33.3060
18	243.5145	36.2406	63.6862
19	131.7695	74.8076	146.6940
20	63.5145	143.7594	116.3138
21	131.7695	74.8076	326.6940
22	243.5145	36.2406	243.6862
23	311.7695	105.1924	213.3060
24	63.5145	143.7594	296.3138

c. Plot the points as a 3D plot (Euler angle space) and show 2 or 3 different views. It is good practice to control the axes so that the 1st and 3rd angles range from 0 to 360° and the 2nd 0 to 180°. The following Matlab commands worked for me, where {x,y,z} are vectors of equal length containing the Euler angle values:

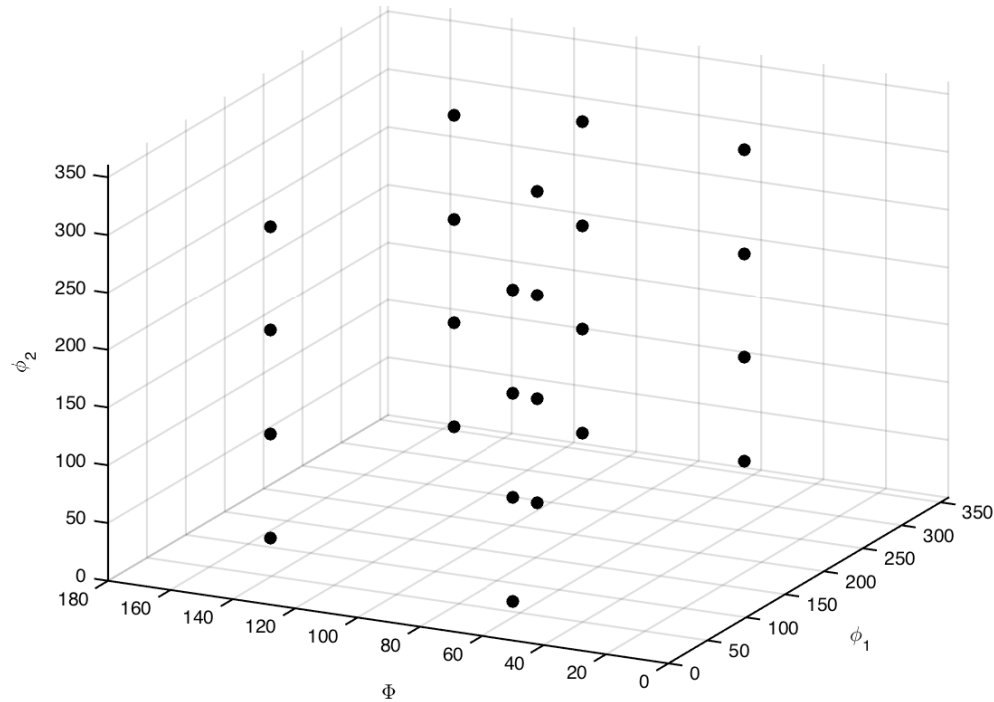
```
scatter3(x,y,z,'MarkerFaceColor','r');
axis([0 360 0 180 0 360]);
xlabel('\phi_1');
ylabel('\Phi');
zlabel('\phi_2');
```

The backslash (" \backslash ") in front of e.g. "Phi" tells Matlab to treat the following letters as a symbol.

View 1



View 2



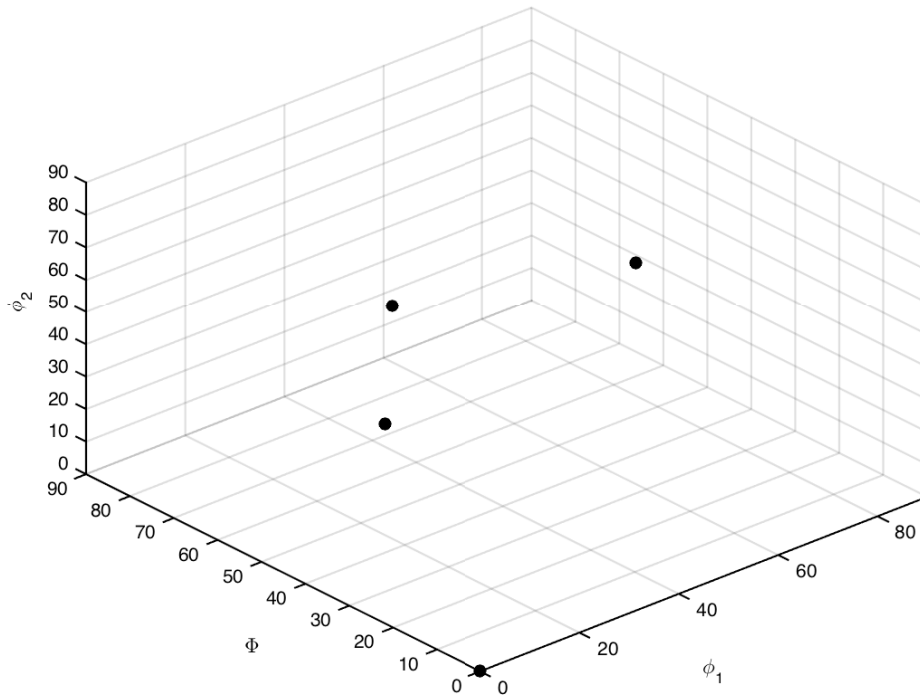
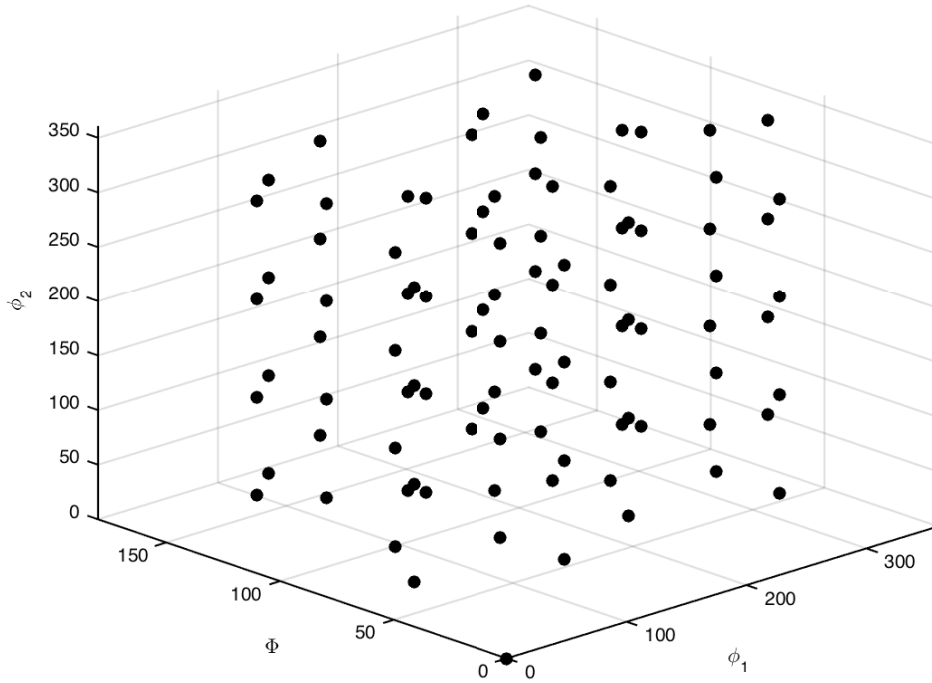
d. Now apply orthorhombic sample symmetry (222 point group) in addition to cubic crystal symmetry (432 point group) and re-draw. Make two views, one with the full range of Euler angles, and a second one with the range limited to 0-90° for all 3 angles.

Used variants_xtal_sample.m (in Matlab)

i	j	phi1	PHI	phi2	(degrees)
1	1	32.0000	58.0000	18.0000	
1	2	148.0000	122.0000	198.0000	
1	3	328.0000	122.0000	198.0000	
1	4	212.0000	58.0000	18.0000	
2	1	212.0000	122.0000	162.0000	
2	2	328.0000	58.0000	342.0000	
2	3	148.0000	58.0000	342.0000	
2	4	32.0000	122.0000	162.0000	
3	1	243.5145	36.2406	153.6862	
3	2	296.4855	143.7594	333.6862	
3	3	116.4855	143.7594	333.6862	
3	4	63.5145	36.2406	153.6862	
4	1	63.5145	143.7594	26.3138	
4	2	116.4855	36.2406	206.3138	
4	3	296.4855	36.2406	206.3138	
4	4	243.5145	143.7594	26.3138	
5	1	212.0000	122.0000	342.0000	

5	2	328.0000	58.0000	162.0000
5	3	148.0000	58.0000	162.0000
5	4	32.0000	122.0000	342.0000
6	1	32.0000	58.0000	198.0000
6	2	148.0000	122.0000	18.0000
6	3	328.0000	122.0000	18.0000
6	4	212.0000	58.0000	198.0000
7	1	63.5145	143.7594	206.3138
7	2	116.4855	36.2406	26.3138
7	3	296.4855	36.2406	26.3138
7	4	243.5145	143.7594	206.3138
8	1	243.5145	36.2406	333.6862
8	2	296.4855	143.7594	153.6862
8	3	116.4855	143.7594	153.6862
8	4	63.5145	36.2406	333.6862
9	1	32.0000	58.0000	108.0000
9	2	148.0000	122.0000	288.0000
9	3	328.0000	122.0000	288.0000
9	4	212.0000	58.0000	108.0000
10	1	311.7695	105.1924	123.3060
10	2	228.2305	74.8076	303.3060
10	3	48.2305	74.8076	303.3060
10	4	131.7695	105.1924	123.3060
11	1	212.0000	122.0000	72.0000
11	2	328.0000	58.0000	252.0000
11	3	148.0000	58.0000	252.0000
11	4	32.0000	122.0000	72.0000
12	1	131.7695	74.8076	56.6940
12	2	48.2305	105.1924	236.6940
12	3	228.2305	105.1924	236.6940
12	4	311.7695	74.8076	56.6940
13	1	32.0000	58.0000	288.0000
13	2	148.0000	122.0000	108.0000
13	3	328.0000	122.0000	108.0000
13	4	212.0000	58.0000	288.0000
14	1	131.7695	74.8076	236.6940
14	2	48.2305	105.1924	56.6940
14	3	228.2305	105.1924	56.6940
14	4	311.7695	74.8076	236.6940
15	1	212.0000	122.0000	252.0000
15	2	328.0000	58.0000	72.0000
15	3	148.0000	58.0000	72.0000
15	4	32.0000	122.0000	252.0000
16	1	311.7695	105.1924	303.3060
16	2	228.2305	74.8076	123.3060
16	3	48.2305	74.8076	123.3060
16	4	131.7695	105.1924	303.3060
17	1	311.7695	105.1924	33.3060

17	2	228.2305	74.8076	213.3060
17	3	48.2305	74.8076	213.3060
17	4	131.7695	105.1924	33.3060
18	1	243.5145	36.2406	63.6862
18	2	296.4855	143.7594	243.6862
18	3	116.4855	143.7594	243.6862
18	4	63.5145	36.2406	63.6862
19	1	131.7695	74.8076	146.6940
19	2	48.2305	105.1924	326.6940
19	3	228.2305	105.1924	326.6940
19	4	311.7695	74.8076	146.6940
20	1	63.5145	143.7594	116.3138
20	2	116.4855	36.2406	296.3138
20	3	296.4855	36.2406	296.3138
20	4	243.5145	143.7594	116.3138
21	1	131.7695	74.8076	326.6940
21	2	48.2305	105.1924	146.6940
21	3	228.2305	105.1924	146.6940
21	4	311.7695	74.8076	326.6940
22	1	243.5145	36.2406	243.6862
22	2	296.4855	143.7594	63.6862
22	3	116.4855	143.7594	63.6862
22	4	63.5145	36.2406	243.6862
23	1	311.7695	105.1924	213.3060
23	2	228.2305	74.8076	33.3060
23	3	48.2305	74.8076	33.3060
23	4	131.7695	105.1924	213.3060
24	1	63.5145	143.7594	296.3138
24	2	116.4855	36.2406	116.3138
24	3	296.4855	36.2406	116.3138
24	4	243.5145	143.7594	296.3138



e. How many points are listed in the new table?

$24 \cdot 4 = 96$.

f. How many of the points lie within the range $0-90^\circ$ for all three angles?

Three.

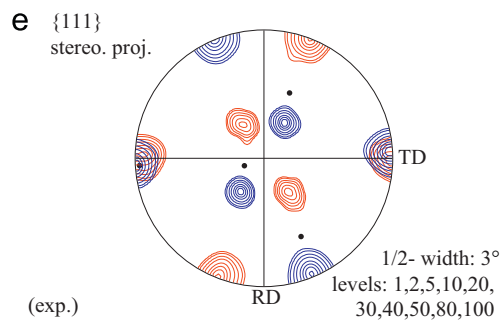
4. [15 points]

This question, and the one following are intended to develop your skills for interpreting pole figures.

a. [10] What sample symmetry does the following pole figure have, which is taken from a recent paper on texture (Quey et al. *J. Mech. Phys. Solids* **60** (2012) 509–524), if you include both the red and blue peaks?

b. [5] What sample symmetry is present if we only consider, say, the red peaks?

(a) The red and blue peaks taken together define an orthorhombic sample symmetry to high accuracy. If (b), we take only the red peaks then the only remaining symmetry is a diad (180° rotation) on the sample Z-axis, i.e. monoclinic sample symmetry.



Appendix

The following fortran90 code shows how to generate the 24 symmetry operators that belong to the (432) point group and that describe cubic crystal symmetry. Note that the first 6 lines of code specify the entries are all zero; the code that follows then changes the appropriate entries in each matrix to 1. This is more reliable than writing out (or assigning) each and every value. An exclamation point means that all characters after that (to the right of the !) are treated as a comment.

Note that all 24 matrices are listed in the Kocks-Tomé-Wenk book and in the lecture notes (and can be copied directly from there).

```
DO I=1,3
  DO J=1,3
    DO K=1,24
      SYM(I,J,K)=0.
    end do
  end do
end do
```

```
! 1
SYM(1,1,1)=1.
SYM(2,2,1)=1.
SYM(3,3,1)=1.
! 5
SYM(1,1,2)=1.
SYM(2,3,2)=-1.
SYM(3,2,2)=1.
! 2
SYM(1,1,3)=1.
SYM(2,2,3)=-1.
SYM(3,3,3)=-1.
! 11
SYM(1,1,4)=1.
SYM(2,3,4)=1.
SYM(3,2,4)=-1.
! 7
SYM(1,3,5)=-1.
SYM(2,2,5)=1.
SYM(3,1,5)=1.
! 12
SYM(1,3,6)=1.
SYM(2,2,6)=1.
SYM(3,1,6)=-1.
! 3
SYM(1,1,7)=-1.
SYM(2,2,7)=1.
SYM(3,3,7)=-1.
! 4
SYM(1,1,8)=-1.
SYM(2,2,8)=-1.
SYM(3,3,8)=1.
! 13
SYM(1,2,9)=1.
SYM(2,1,9)=-1.
SYM(3,3,9)=1.
! 6
SYM(1,2,10)=-1.
SYM(2,1,10)=1.
SYM(3,3,10)=1.
! 20
SYM(1,2,11)=-1.
SYM(2,3,11)=1.
SYM(3,1,11)=-1.
! 23
SYM(1,3,12)=1.
SYM(2,1,12)=-1.
```

SYM(3,2,12)=-1.
! 19
SYM(1,2,13)=-1.
SYM(2,3,13)=-1.
SYM(3,1,13)=1.
! 21
SYM(1,3,14)=-1.
SYM(2,1,14)=1.
SYM(3,2,14)=-1.
! 18
SYM(1,2,15)=1.
SYM(2,3,15)=-1.
SYM(3,1,15)=-1.
! 22
SYM(1,3,16)=-1.
SYM(2,1,16)=-1.
SYM(3,2,16)=1.
! 9
SYM(1,2,17)=1.
SYM(2,3,17)=1.
SYM(3,1,17)=1.
! 8
SYM(1,3,18)=1.
SYM(2,1,18)=1.
SYM(3,2,18)=1.
! 17
SYM(1,2,19)=1.
SYM(2,1,19)=1.
SYM(3,3,19)=-1.
! 24
SYM(1,1,20)=-1.
SYM(2,3,20)=1.
SYM(3,2,20)=1.
! 10
SYM(1,3,21)=1.
SYM(2,2,21)=-1.
SYM(3,1,21)=1.
! 15
SYM(1,1,22)=-1.
SYM(2,3,22)=-1.
SYM(3,2,22)=-1.
! 16
SYM(1,3,23)=-1.
SYM(2,2,23)=-1.
SYM(3,1,23)=-1.
! 14
SYM(1,2,24)=-1.
SYM(2,1,24)=-1.

$$\text{SYM}(3, 3, 24) = -1.$$