

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.

- a. 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);
- b. 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;
- 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;
- e. Compute the coefficients of this same vector in the new, primed frame;
- 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.

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

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.

- a. Draw the same x-y frame;

- b. Draw the same unit vector parallel to [410] as above;
- c. Write out the transpose of the transformation matrix that you obtained above, which is the matrix that represents the corresponding rotation.
- d. Compute and draw the new rotated vector.

3. [30]

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.

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).

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');
% makes 3D plot, click on the rotation button to control the viewpoint
axis([0 360 0 180 0 360]); % sets the axis lengths
xlabel('\phi_1');
ylabel('\Phi');
zlabel('\phi_2');
```

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

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.

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

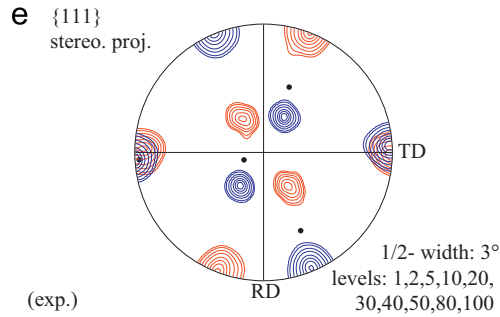
f. How many of the points lie within the range 0-90° for all three angles?

4. [15]

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?



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.
SYM(3,3,24)=-1.
```