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3.012 Fundamentals of Materials Science and Engineering – Fall 2003

Problem Set Five: Structure Solutions

Problem 1

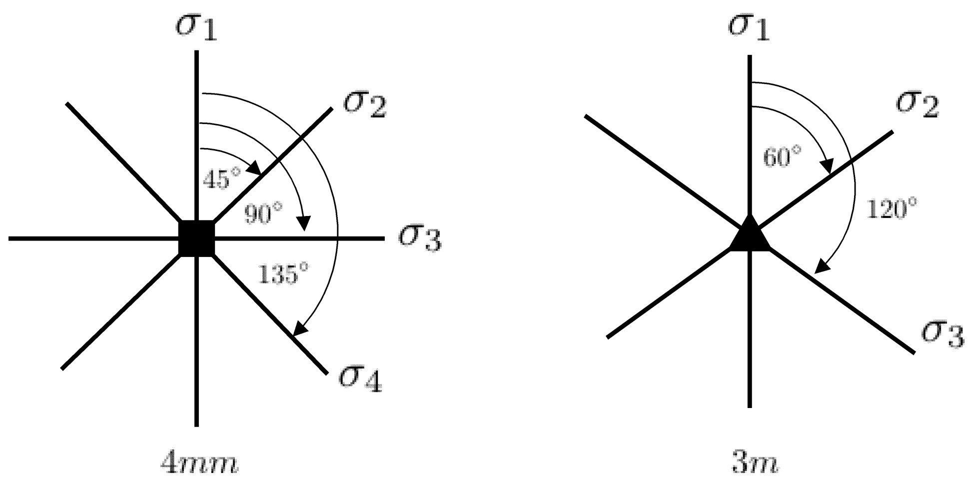

Figure 1: Point groups 4mm and 3m

Let's compare point groups 3m and 4mm.

- In 4mm, $\sigma_1$and $\sigma_3$are related by the 90 degree rotation of the 4-fold axis. Said another way, by placing in $\sigma_1$we obtain $\sigma_3$by the operation on the 4-fold axis on it. But you also get $\sigma_2$and $\sigma_4$when you combine $\sigma_1$with a perpendicular rotation axes using the combination relations we discussed in class.

$\sigma_1 \bullet A_{\frac{\pi}{2}} = \sigma_2$	with the angle between the planes being 90/2 or 45 degrees
$\sigma_1 \bullet A_{\pi} = \sigma_3$	we already had this one, another mirror 90 degrees away
$\sigma_1 \bullet A_{\frac{3\pi}{2}} = \sigma_4$	with the angle between the planes being 270/2 or 135 degrees

  There are then two distinct sets of mirror planes: σ_1& $\sigma_3$and σ_2& σ_4. Theae two sets are not equivalent since the operation of the rotation axis (4-fold) will never map the two sets to the same location. Thus we call this group 4mm.

- In 3m when we place in the first mirror plane, σ_1, we get two more planes due to the operation of the rotation axis. ($\sigma_2$and σ_3). But like 4mm we should also see if the combination of the operations of the rotation axis and the mirror plane produce any more mirrors.

$\sigma_1 \bullet A_{\frac{2\pi}{3}} = \sigma_2$	with the angle between the planes being 120/2 or 60 degrees
$\sigma_1 \bullet A_{\frac{4\pi}{3}} = \sigma_3$	with the angle between the planes being 240/2 or 120 degrees

  But we already have these planes due to the operation of the 3-fold axis. Therefore, there is only one kind of distinct mirror plane here, and we call this group 3m.

Problem 2

(a)

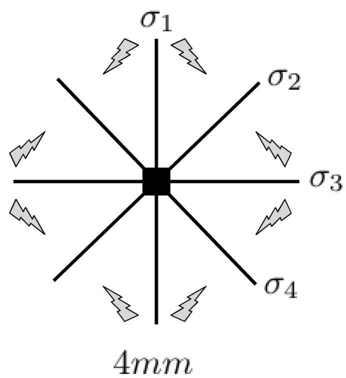

Figure 2: The pattern of motifs associated with point group 4mm

(b)

$4mm$ consists of the following operations: $\{A_{\frac{\pi}{2}}$, A_{π}, $A_{\frac{3\pi}{2}}$, $A_{2\pi}$, σ_1, σ_2,σ_3, $\sigma_4\}$. The group multiplication table would look something like this:

	$A_{\frac{\pi}{2}}$	A_{π}	$A_{\frac{3\pi}{2}}$	$A_{2\pi}$	σ_1	σ_2	σ_3	σ_4
$A_{\frac{\pi}{2}}$	A_{π}	$A_{\frac{3\pi}{2}}$	$A_{2\pi}$	$A_{\frac{\pi}{2}}$	σ_2	σ_3	σ_4	σ_1
A_{π}	$A_{\frac{3\pi}{2}}$	$A_{2\pi}$	$A_{\frac{\pi}{2}}$	A_{π}	σ_3	σ_4	σ_1	σ_2
$A_{\frac{3\pi}{2}}$	$A_{2\pi}$	$A_{\frac{\pi}{2}}$	A_{π}	$A_{\frac{3\pi}{2}}$	σ_4	σ_1	σ_2	σ_3
$A_{2\pi}$	$A_{\frac{\pi}{2}}$	A_{π}	$A_{\frac{3\pi}{2}}$	$A_{2\pi}$	σ_1	σ_2	σ_3	σ_4
σ_1	σ_4	σ_3	σ_2	σ_1	$A_{2\pi}$	$A_{\frac{3\pi}{2}}$	A_{π}	$A_{\frac{\pi}{2}}$
σ_2	σ_1	σ_4	σ_3	σ_2	$A_{\frac{\pi}{2}}$	$A_{2\pi}$	$A_{\frac{3\pi}{2}}$	A_{π}
σ_3	σ_2	σ_1	σ_4	σ_3	A_{π}	$A_{\frac{\pi}{2}}$	$A_{2\pi}$	$A_{\frac{3\pi}{2}}$
σ_4	σ_3	σ_2	σ_1	σ_4	$A_{\frac{3\pi}{2}}$	A_{π}	$A_{\frac{\pi}{2}}$	$A_{2\pi}$

In constructing the table the order of operations that I used was first I performed the operation in the left column, then I performed the operation from the top row. This is important to note because not every set of operations can commute. For example (see figure 3 on the next page):

$$A_{\frac{\pi}{2}} \bullet \sigma_1 \neq \sigma_1 \bullet A_{\frac{\pi}{2}}$$

Does this meet the three requirements needed to define a group?

1. Every combination of elements is also a member of the group. *This checks out. When we complete the multiplication table, we only see members of the group. We do not get any new operations.*

2. For every element there is an inverse. *This checks out too. For every operation in the group we can find another element for which when you combine them we get the identity element ($A_{2\pi}$).*

3. The identity operation is present. *Okay here as well. Looking at the multiplication table we can see that $A_{2\pi}$is out identity element since any other element combined with $A_{2\pi}$gives us the element back again. ($A_{2\pi}\bullet X = X$)*

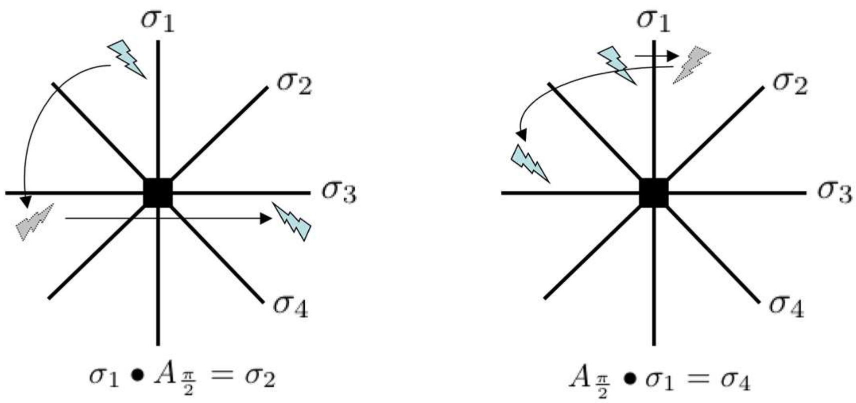

Figure 3: The order of operations is important

(c)

There are 8 motifs in the pattern and the rank of the group (the number of operations) is also 8!

Problem 4

(a)

A rotation of 90 degrees ($\frac{\pi}{2}$) about $x_2$would look like this:

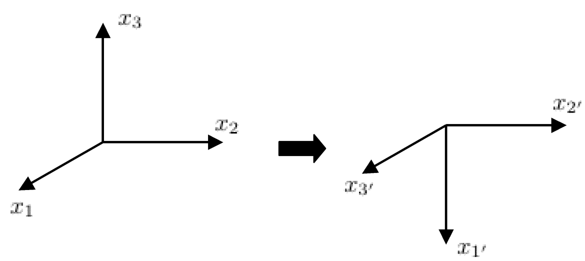

Figure 4: A rotation of 90 degrees about x_2

So the transformation of the axes would go something like this:

$$\begin{aligned} x_1' &= && && -x_3 \\ x_2' &= && x_2 && \\ x_3' &= -x_1 && && \end{aligned}$$

And the direction cosine would look like this:

$$c_{ij} = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}$$

(b)

A reflection in the x_1-x_2 plane would look like this:

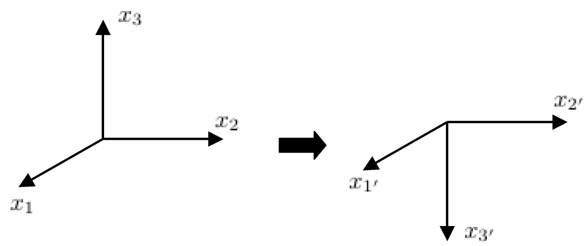

Figure 5: A reflection in the x_1-x_2 plane

So the transformation of the axes would go something like this:

$$\begin{array}{lcccc} x_1' & = & x_1 & & \\ x_2' & = & & x_2 & \\ x_3' & = & & & -x_3 \end{array}$$

And the direction cosine would look like this:

$$c_{ij} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

(c)

Looking down at a cube along the [111] direction we would see something like the figure below. (This view makes it easier to see the 3-fold symmetry possessed by a cube).

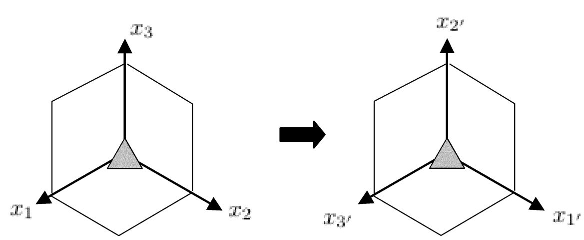

Figure 6: Rotation by 120 degrees about the [111] direction of a cubic crystal. The triangle idicates the location of a 3-fold axis.

So the transformation of the axes would go something like this:

$$\begin{array}{lcccc} x_1' & = & & x_2 & \\ x_2' & = & & & x_3 \\ x_3' & = & x_1 & & \end{array}$$

And the direction cosine would look like this:

$$c_{ij} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

Problem 5

Inversion will take xyz and transform it into $\bar{x}\bar{y}\bar{z}$. So to get our direction cosine for this transformation we can write:

$$\begin{array}{lllll} x_1' & = & -x_1 & & \\ x_2' & = & & -x_2 & \\ x_3' & = & & & -x_3 \end{array}$$

And the direction cosine would look like this:

$$c_{ij} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

We can see from this that if $i = j$ then $c_{ij} = -1$ and if $i \neq j$ then $c_{ij} = 0$. This makes the transformation much easier. We can write:

$$\sigma_{ij}' = c_{il}c_{jm}\sigma_{ij}$$

$$\sigma_{ij}' = c_{ii}c_{jj}\sigma_{ij}$$

$$\sigma_{ij}' = (-1)(-1)\sigma_{ij}$$

$$\sigma_{ij}' = \sigma_{ij}$$

Which doesn't place any restriction on the form of the second rank tensor σ_{ij}.