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3.012 Fundamentals of Materials Science and Engineering – Fall 2003

Example Problems From Recitation (Week of 10/6/03)

Problem 1: Statement

A tetragonal crystal has three orthogonal axes with lattice constants a_1, a_2, and c equal to 3, 3, and 7 $\mathring{A}$ respectively.

(a) Make a sketch of one or more unit cells of this crystal and outline planes with Miller indices of (110), $(3\bar{2}1)$, and $(0\bar{1}1)$.

(b) Find the angles between each of these pairs of directions in this tetragonal crystal:

1. $[110]$ and $[1\bar{1}0]$
2. $[110]$ and $[10\bar{1}]$
3. $[100]$ and $[111]$

Problem 1: Solution

Part (a)

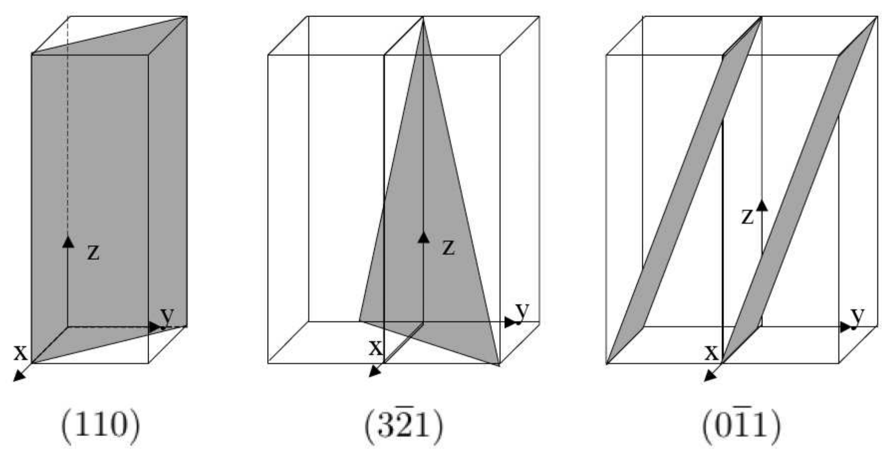

Figure 1: Planes for part (a)

Part (b)

To find the angles between the direction we can use the dot product since the axes are orthogonal. However, since it is a tetragonal crystal, all the axes are not the same length. We must scale them with the correct values for the lattice constants.

1.

$$A = [110] = a\hat{x} + a\hat{y} + 0\hat{z}$$

$$B = [1\bar{1}0] = a\hat{x} - a\hat{y} + 0\hat{z}$$

$$A \cdot B = a^2 - a^2 - 0$$

We can find the angle since we also know that:

$$A \cdot B = |A||B| \cos\theta$$

$$0 = |A||B| \cos\theta \rightarrow \cos\theta = 0$$

$$\theta = 90^\circ$$

2.

$$A = [110] = a\hat{x} + a\hat{y} + 0\hat{z}$$

$$B = [10\bar{1}] = a\hat{x} - 0\hat{y} - c\hat{z}$$

$$A \cdot B = a^2$$

$$a^2 = |A||B| \cos\theta = (\sqrt{2a^2})(\sqrt{a^2 + c^2}) \cos\theta$$

$$\theta = \cos^{-1}\left[\frac{a^2}{(a\sqrt{2})(\sqrt{a^2 + c^2})}\right] = \cos^{-1}\left[\frac{3^2}{(3\sqrt{2})(\sqrt{3^2 + 7^2})}\right]$$

$$\theta = \cos^{-1}(0.27853)$$

$$\theta = 73.83^\circ$$

3.

$$A = [100] = a\hat{x} + 0\hat{y} + 0\hat{z}$$

$$B = [111 = a\hat{x} + a\hat{y} + c\hat{z}$$

$$A \cdot B = a^2$$

$$a^2 = |A||B| \cos\theta = (a\sqrt{2a^2 + c^2}) \cos\theta$$

$$\theta = \cos^{-1}\left[\frac{a^2}{(a\sqrt{2a^2 + c^2})}\right] = \cos^{-1}\left[\frac{3^2}{(3\sqrt{2 * 3^2 + 7^2})}\right]$$

$$\theta = \cos^{-1}(0.36650)$$

$$\theta = 68.50^\circ$$

Problem 2: Statement

The first three diffraction peaks of a metal powder are $2\theta = 44.4°, 64.6°, 81.7°$ using CuK$_\alpha$-radiation ($\lambda = 1.542\mathring{A}$). Is the metal Cr, Ni, Ag, or W?

Problem 2: Solution

First we need to look up the crystal structures and lattice constants for these four metals.

Cr	BCC	$2.885\mathring{A}$
Ni	FCC	$3.524\mathring{A}$
Ag	FCC	$4.806\mathring{A}$
W	BCC	$3.165\mathring{A}$

We know the relationship between λ, d, and θ, its just Bragg's Law:

$$\lambda = 2d_{hkl}\sin\theta$$

And we also know that for a cubic crystal the interplanar spacing is related to h, k, and l by:

$$d = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

Putting that together we get:

$$\lambda = 2\left(\frac{a}{\sqrt{h^2+k^2+l^2}}\right)\sin\theta$$

$$a = \frac{\lambda(\sqrt{h^2+k^2+l^2})}{2\sin\theta}$$

Now we have to figure out what are the first three reflections in BCC and FCC

Reflection	BCC (h+k+l=even)	FCC (h,k,l all even or all odd)
1	110	111
2	200	200
3	211	220

Now for each crystal system, lets plug in our values of θ for each reflection and find out what the lattice parameter should be. Starting with FCC, the first reflection would be 111, so:

$$a = \frac{1.542(\sqrt{1^2+1^2+1^2})}{2\sin(22.2)°} = 3.534\mathring{A}$$

This is pretty close to the lattice constant for Ni, but we have to try the next reflection to make sure these reflections would be consistent with an FCC crystal. The next reflection would be 200:

$$a = \frac{1.542(\sqrt{2^2+0^2+0^2})}{2\sin(32.3)°} = 2.8856\mathring{A}$$

Uh oh! These two values do not match, meaning that these reflection cannot be from an FCC crystal. Let's try BCC. The first reflection there would be 110:

$$a = \frac{1.542(\sqrt{1^2 + 1^2 + 0^2})}{2\sin(22.2)^\circ} = 2.8858\mathring{A}$$

This is pretty close to the lattice constant of Cr. Let's continue and do the other two reflections just to make sure. Second we would have 200:

$$a = \frac{1.542(\sqrt{2^2 + 0^2 + 0^2})}{2\sin(32.3)^\circ} = 2.8856\mathring{A}$$

This is still consistent with the first reflection. Finally we would have 211:

$$a = \frac{1.542(\sqrt{2^2 + 1^2 + 1^2})}{2\sin(40.85)^\circ} = 2.8873\mathring{A}$$

Thats pretty close. It would be safe to say that this metal is BCC and is most likely Cr.