Introduction to Crystallography (Homework No. 2)

Due Date: September 17, 2008

1. What is the condition for an (hkl) plane to contain the line $[\bar{2}31]$?

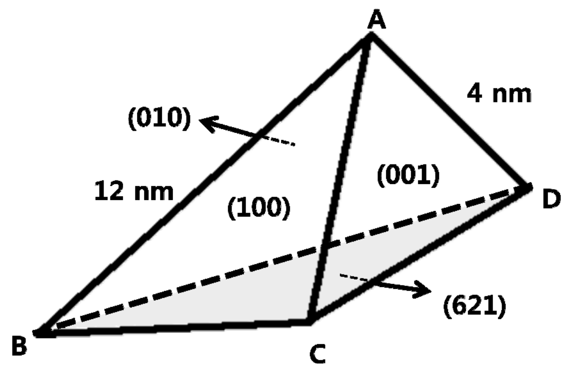
2. Answer the following questions.

(a) Sketch a cubic system and draw in the plane (110) and line [110]. Are they perpendicular?

(b) Repeat (a) in an orthorhombic system. Are they perpendicular?

(c) Now we can see that [hkl] isn't necessarily perpendicular to (hkl). (This is one of the reasons why we need reciprocal lattice vectors.) What would be the condition required for [110] to be perpendicular to (110)?

(d) Which crystal systems fulfill these conditions?



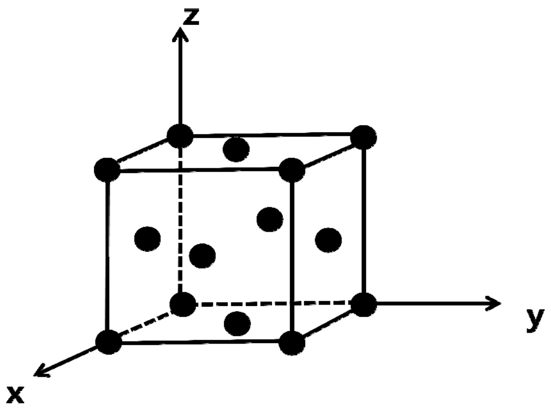
Prob. 3

3. Consider a nano-crystallite as depicted above. [ABD=(010), ABC=(100), ADC=(001), BCD=(621), $\overline{AB}$ = 12 nm, $\overline{AD}$ = 4 nm] Since this is a crystal, you would expect atoms to be ordered inside the crystallite. This crystal is known to have a triclinic system (primitive), and the atomic distance along the a_1, a_2, a_3 axis is 2Å, 1.5Å, 1Å respectively.

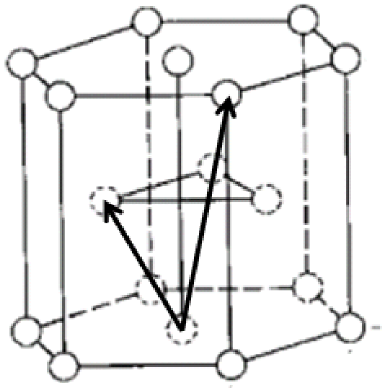
(a) What is the crystalline direction of $\overline{AB}, \overline{AC}$ and $\overline{AD}$?

(b) What would be the length of $\overline{AC}$?

(c) Calculate the number of planes parallel to the shaded bottom-surface.



Prob. 4



Prob. 5

4. In class, you have seen how the reciprocal lattice of a BCC lattice becomes an FCC lattice. Here, we shall see which type of lattice is reciprocal to FCC.

(a) Consider an FCC unit cell with a lattice constant a_0. To obtain the correct reciprocal lattice, you will need lattice vectors of a primitive cell. A convenient choice would be

$$\vec{a}_p = \frac{a_0}{2}(\hat{y}+\hat{z}),\ \vec{b}_p = \frac{a_0}{2}(\hat{z}+\hat{x}),\ \vec{c}_p = \frac{a_0}{2}(\hat{x}+\hat{y})$$

Indicate these vectors on the FCC unit cell and see how it defines a primitive unit cell.

(b) From these vectors, obtain reciprocal vectors $\vec{a}^*_p$, $\vec{b}_p^*$, $\vec{c}^*_p$.

(c) With the $\vec{a}^*_p$, $\vec{b}_p^*$, $\vec{c}^*_p$ vectors you have obtained, construct a space lattice with xyz axes indicated. (In class, you have learned how a space lattice is constructed through translation.) Figure out the lattice type.

(d) Now you may think that the reciprocal lattice of the reciprocal lattice of any lattice is eventually the original lattice itself. Indeed, if one lattice is reciprocal to another, the relation holds vice versa. Try proving this by showing that the reciprocal vector of $\vec{a}^*$ becomes $\vec{a}$.

Hint : solve the following

$$\frac{\vec{b}^* \times \vec{c}^*}{\vec{a}^* \bullet (\vec{b}^* \times \vec{c}^*)}$$

Try substituting $\vec{a}^*$ and one $\vec{c}^*$ with original vectors, and use the vector relationship

$$\vec{a} \times (\vec{b} \times \vec{c}) = (\vec{a} \bullet \vec{c})\vec{b} - (\vec{a} \bullet \vec{b})\vec{c}$$

5. Consider an HCP lattice. Calculate the angle between the two directions indicated.
Assume, c/a=1.6.