HW 3

Levon Dovlatyan, SI: 24451582
E45

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Problem 3.3. Why is there no base-centered cubic lattice in Table 3.2? (Use a sketch to answer)

By placing several base-centered cubics side by side and looking at cross sectional view, we can see why there is no need for a base-centered cubic. The unit cell of a base-centered cubic can be draw using the center base-centered points as will which would make it a simple tetragonal. So a base-centered cubic is infact just a tetragonal, hence there is no need for one.

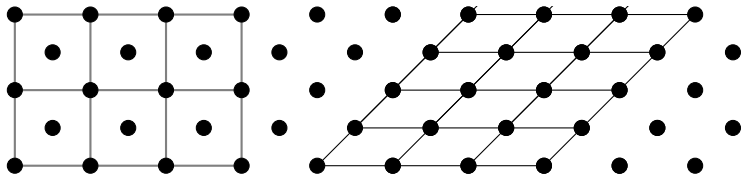


Figure 1: A set of lattice points showing the cross-sectional view of several base-centered cubics.

Problem 3.7. Calculate the density of Mg, an hcp metal. (Note Problem 3.11 for the ideal c.a ratio.)

The volume of a hexagonal is $V = h * A$ where h is the height and A is the area of the base. The area of the base is $A = a^2 * \sin 60$ where a is the edge length. The height of the hexagonal is related to the edge length where $h = 1.633 * a$. For an hcp, $a = 2r_{Mg}$ where $r_{Mg} = 0.160$ nm.

$$\rho = \frac{2\,\text{atoms}}{h * A} = \frac{2\,\text{atoms}}{1.633a^3 \sin 60} = \frac{2\,\text{atoms}}{1.633 \sin 60 (0.32 \times 10^{-9}\,\text{m})^3} * \frac{24.31\,\text{g}}{6.023 \times 10^{23}\,\text{atoms}} * (\frac{1\,\text{m}}{10^2\,\text{cm}})^3$$
$$= 1.74\,\text{g/cm}^3$$

Problem 3.10. Calculate the APF of 0.74 for hcp metals.

From the previous problem we know that the volume of an hcp unit cell is $V_{cell} = 1.633\,a^3 \sin 60$ where $a = 2r_{atom}$. The hcp structure also contains 2 full atoms inside it. Using this data we can solve for teh APF.

$$\text{APF} = \frac{V_{atoms}}{V_{cell}} = \frac{2 * (\frac{4\pi}{3} {r_{atom}}^3)}{1.633\,\sin 60 (2r_{atom})^3} = \frac{2\pi}{3\sqrt{3} * 1.633} = 0.74$$

Problem 3.17. Calculate the IPF for cristobalite (Figure 3.11).

$$V_{atoms} = 8(\frac{4\pi {r_{Si^{4+}}}^3}{3}) + 16(\frac{4\pi {r_{O^{2-}}}^3}{3}) = 0.156\,\text{nm}^3$$
$$V_{cube} = a^3 = \frac{d^3}{2^{\frac{3}{2}}} = \frac{(8r_{O^{2-}} + 2r_{Si^{4+}})^3}{2^{\frac{3}{2}}} = 0.516\,\text{nm}^3$$
$$\text{IPF} = \frac{V_{atoms}}{V_{cube}} = \frac{0.156}{0.516} = 0.317$$

Problem 3.27. **(a)** Sketch, in a cubic unit cell, a [111] and a [112] lattice direction. **(b)** Use a trigonometric calculation to determine the angle between these two directions. **(c)** Use Equation 3.3 to determine the angle between these two directions.

(a) This was done in python,

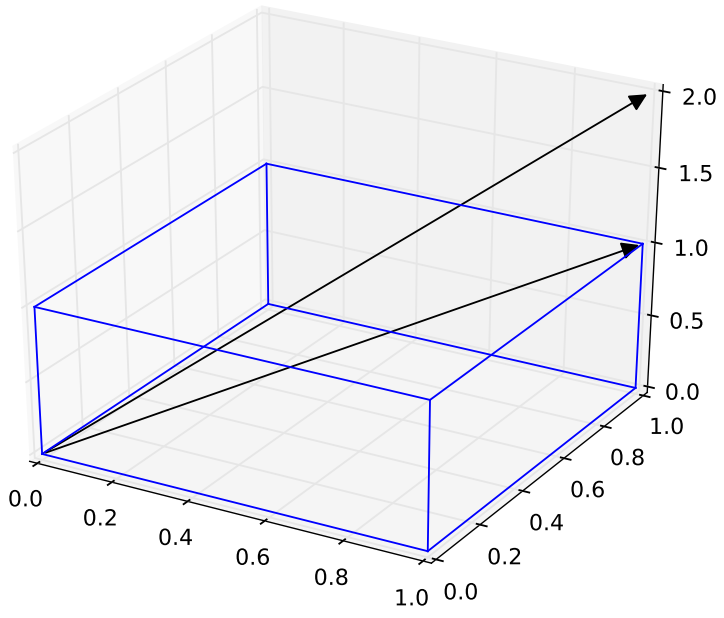
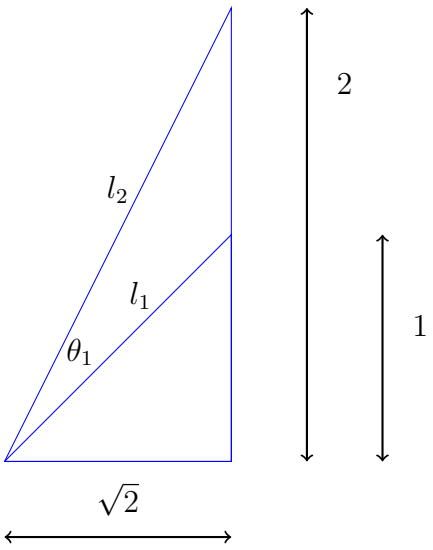


Figure 2: cubic unit cell with vectors [111] and [112]

(b) Using simple geometry we get to this point,



Where l_1 represents the [111] vector and l_2 represents the [112] vector. Using law of cosines we see that $2^2 = {l_1}^2 + {l_2}^2 - 2l_1 l_2 \cos\theta_2$. Where $l_1 = \sqrt{3}$ and $l_2 = \sqrt{6}$. Pluggin this in, we get $\theta_1 = \arccos\frac{4}{\sqrt{18}} \approx 19.5$ degrees.

(c)

$$V_1 = (1,1,1), \;\; V_2 = (1,1,2)$$

$$\cos\theta = \frac{V_1 \dot{V}_2}{|V_1||V_2|} = \frac{1*1+1*1+1*2}{\sqrt{1^2+1^2+1^2}\sqrt{1^2+1^2+2^2}} = \frac{4}{\sqrt{18}}$$

This is the same as part b, the answer is $\theta \approx 19.5$ degrees.