, ×5 = 25 points

HW #1 solutions

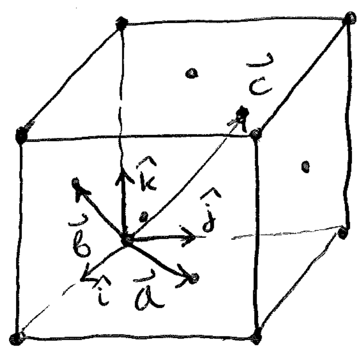
Physics 406

(1.) O. Ch. 1, Pr. 1

The primitive basis vectors are

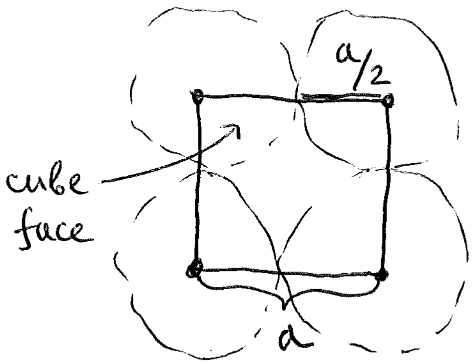
$$\begin{cases} \vec{a} = \left(\frac{a}{2}, \frac{a}{2}, 0\right), \\ \vec{b} = \left(0, \frac{a}{2}, \frac{a}{2}\right), \\ \vec{c} = \left(\frac{a}{2}, 0, \frac{a}{2}\right) \end{cases}$$

The Bravais lattice is fcc: all points in the fcc lattice are linear combinations of $\vec{a}, \vec{b}, \vec{c}$:



(2.) O. Ch. 1, Pr. 4

sc: $r_{sc} = \frac{a}{2}$, $V_{sc} = \frac{4\pi}{3}\left(\frac{a}{2}\right)^3$

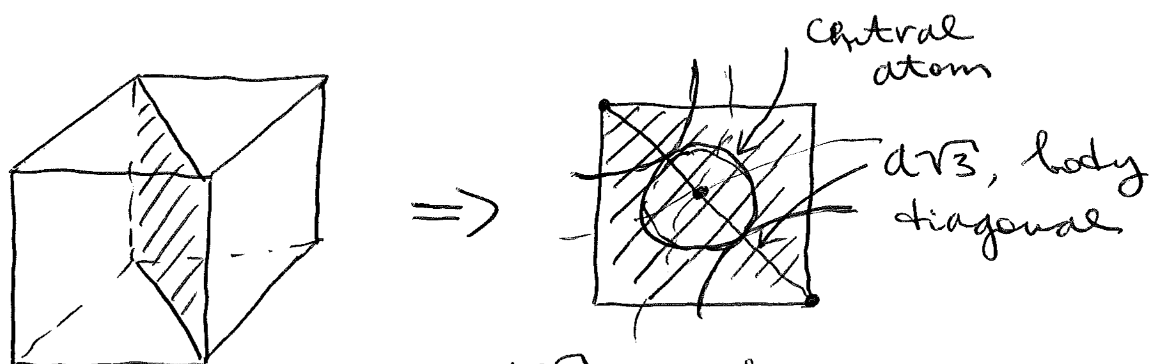


1 atom per unit cell:

packing ratio

$$P_f^{sc} = \frac{4\pi}{3}\left(\frac{a}{2}\right)^3 \frac{1}{a^3} = \frac{\pi}{6} \simeq 0.52$$

bcc:

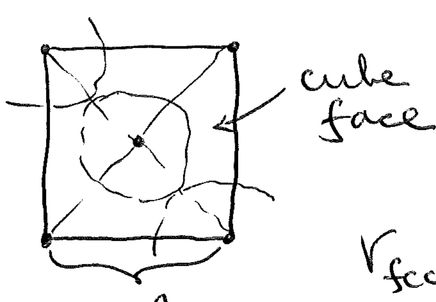


$r_{bcc} = \frac{a\sqrt{3}}{4}$ (spheres touch on the body diagonal)

Note that $r_{bcc} < r_{sc}$, but there are 2 atoms per unit cell:

$$P_f^{bcc} = 2 \times \frac{4\pi}{3}\left(\frac{a\sqrt{3}}{4}\right)^3 \frac{1}{a^3} = \frac{\pi\sqrt{3}}{8} \simeq 0.68 > P_f^{sc}$$

fcc:



$r_{fcc} = \frac{a\sqrt{2}}{4}$ (spheres touch on the face diagonal)

$r_{fcc} < r_{bcc}$, but with 4 atoms per unit cell,

$$P_f^{fcc} = 4 \times \frac{4\pi}{3}\left(\frac{a\sqrt{2}}{4}\right)^3 \frac{1}{a^3} = \frac{\pi\sqrt{2}}{6} \simeq 0.74 > P_f^{bcc}$$

ideal packing ratio

(3.) The bcc lattice has $V = a^3$ & 2 atoms per unit cell. Thus the volume of the primitive unit cell is $a^3/2$.

Similarly, the fcc lattice has $V = a^3$ & 4 atoms per unit cell. Thus the volume of the primitive unit cell is $a^3/4$.

(4.) Intercepts are $(4, 2, \bar{3})$.

Reciprocals are $\left(\frac{1}{4}, \frac{1}{2}, \frac{\bar{1}}{3}\right) \Rightarrow$

$\Rightarrow$ the Miller indices are

$$(3\ 6\ \bar{4})$$

The direction normal to this plane is given by $[3, 6, \bar{4}]$.

(5.) (a) C_1 rotation

\ reflection

(b) same as (a)

(c) same as (a), plus

C_2 rotation, C_4 rotation,

/ , | , — reflections,

inversion through the center of the figure.

Only C_1 rotation & \ reflection are shared by all three.