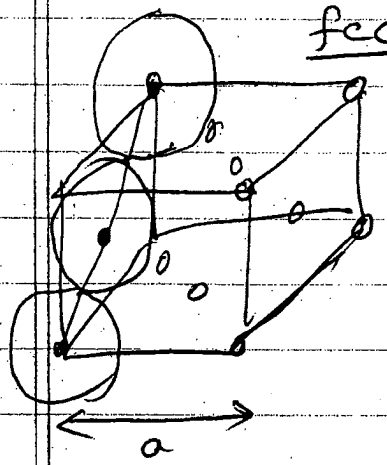
1) Choose radii of spheres so that nearest neighbors touch $\Rightarrow r = \frac{1}{2}$ nearest neighbor distance

fcc



distance between nearest neighbors $= \frac{1}{2}$ the length of the face diagonal

$= \frac{1}{2}\sqrt{2}\,a = \frac{a}{\sqrt{2}}$

So radius $r = \frac{a}{2\sqrt{2}}$

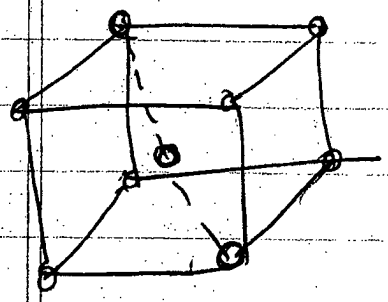
Each of the 8 corner sites contributes $\frac{1}{8}$ of a sphere to the unit cell. Each of the 6 face center sites contributes $\frac{1}{2}$ of a sphere to the unit cell $\Rightarrow$ total of $8\left(\frac{1}{8}\right) + 6\left(\frac{1}{2}\right)$ = 4 spheres per unit cell.

$$\Rightarrow \text{density} = \frac{\text{vol of spheres}}{\text{vol unit cell}} = \frac{4 \cdot \frac{4}{3}\pi r^3}{a^3}$$

$$= \frac{16}{3}\pi \frac{a^3}{8 \cdot 2\sqrt{2}} \frac{1}{a^3} = \frac{\pi}{3\sqrt{2}} = \frac{\sqrt{2}\,\pi}{6}$$

$$\boxed{\text{fcc density} = \frac{\sqrt{2}\,\pi}{6}}$$

bcc



distance between nearest neighbors is $\frac{1}{2}$ the length of the body diagonal

$= \frac{1}{2}\sqrt{3}\,a$

So radius $r = \frac{\sqrt{3}}{4}a$

each of the 8 corner sites gives 1/8 of a sphere to the unit cell. Each body center site gives 1 sphere to the unit cell

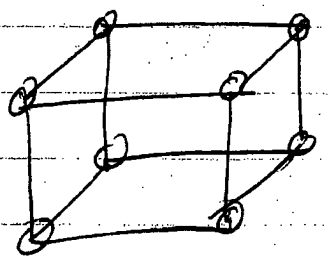
$\Rightarrow$ total of $8(1/8) + 1 = 2$ spheres per unit cell

$$\Rightarrow \text{density} = \frac{\text{vol of spheres}}{\text{vol unit cell}} = \frac{2 \cdot \frac{4}{3}\pi r^3}{a^3}$$

$$= \frac{8}{3}\pi \frac{3\sqrt{3}}{4 \cdot 16} \frac{a^3}{a^3} = \frac{\sqrt{3}\,\pi}{8}$$

$$\boxed{\text{bcc density} = \frac{\sqrt{3}}{8}\pi}$$

sc



distance between nearest neighbors is length of side $= a$

so radius of sphere is $r = \frac{a}{2}$

Each corner site gives $\frac{1}{8}$ of a sphere to the unit cell
$\Rightarrow$ total of $8 \cdot (\frac{1}{8}) = 1$ sphere per unit cell

$$\Rightarrow \text{density} = \frac{\text{vol of sphere}}{\text{vol of unit cell}} = \frac{1 \cdot \frac{4}{3}\pi r^3}{a^3}$$

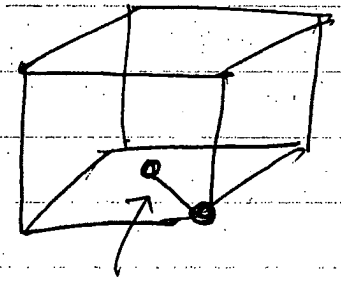
$$= \frac{4\pi}{3}\frac{a^3}{8}\frac{1}{a^3} = \frac{\pi}{6}$$

sc density $= \pi/6$

diamond structure = fcc with 2 point basis

$\vec{d}_1 = 0$, $\vec{d}_2 = \frac{a}{4}(\hat{x} + \hat{y} + \hat{z})$

↑ one quarter of body diagonal



basis vector $\vec{d}_2 = \frac{a}{4}(\hat{x} + \hat{y} + \hat{z})$

nearest neighbor distance is $\frac{1}{4}$ the length of the body diagonal $= \frac{\sqrt{3}a}{4}$

So radius of sphere is $r = \frac{1}{2}\frac{\sqrt{3}a}{4} = \frac{\sqrt{3}}{8}a$

From the fcc sites we get 4 spheres as in part (a). From the $\vec{d}_2$ basis sites we also get 4 spheres per unit cell.
We can see this because the diamond structure is two interpenetrating fcc B.L. so each should contribute the same number of spheres to the unit cell. Or explicitly, the 4 sites
$\vec{d}_2$, $\frac{a}{2}(\hat{x}+\hat{y})+\vec{d}_2$, $\frac{a}{2}(\hat{x}+\hat{z})+\vec{d}_2$, $\frac{a}{2}(\hat{y}+\hat{z})+\vec{d}_2$
all lie with the unit cell. So 8 total spheres

$$\Rightarrow \text{density} = \frac{\text{vol of spheres}}{\text{vol unit cell}} = \frac{8\,\frac{4}{3}\pi r^3}{a^3}$$

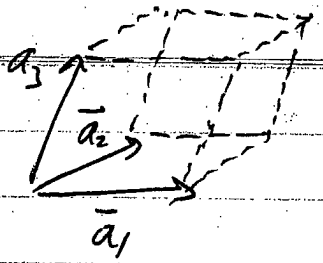
$$= \frac{32\pi}{3}\,\frac{3\sqrt{3}}{8\cdot 64}\,a^3\,\frac{1}{a^3} = \frac{\sqrt{3}}{16}\pi$$

$$\boxed{\text{diamond density} = \frac{\sqrt{3}}{16}\pi}$$

densities are in the order:

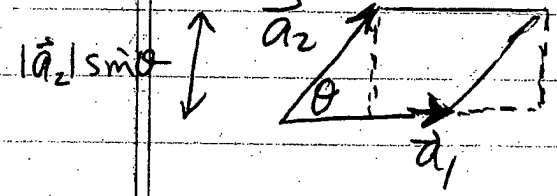
diamond < sc < bcc < fcc

2) a)



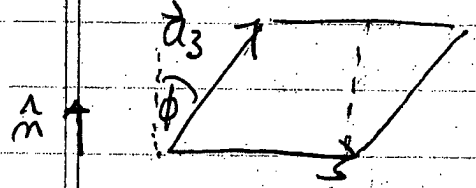
we want the volume of the parallelpiped given by $\vec{a}_1, \vec{a}_2, \vec{a}_3$

consider parrallelogram given by $\vec{a}_1$ and $\vec{a}_2$ in the xy plane



area is $|\vec{a}_1||\vec{a}_2|\sin\theta = |\vec{a}_1 \times \vec{a}_2|$

side view of plane spanned by $\vec{a}_1$ and $\vec{a}_3$



volume of parallelpiped is area of base plane, $|\vec{a}_1 \times \vec{a}_2|$, times $|\vec{a}_3|\cos\phi = \vec{a}_3 \cdot \hat{n}$ where $\hat{n}$ is normal to xy plane spanned by $\vec{a}_1$ and $\vec{a}_2$

$$v = |\vec{a}_1 \times \vec{a}_2||\vec{a}_3|\cos\phi$$

Now $\vec{a}_1 \times \vec{a}_2$ points in direction normal to xy plane i.e. $\vec{a}_1 \times \vec{a}_2 = |\vec{a}_1 \times \vec{a}_2|\hat{n}$

$$\Rightarrow v = |\vec{a}_1 \times \vec{a}_2||\vec{a}_3|\cos\phi$$

$$\boxed{v = |(\vec{a}_1 \times \vec{a}_2) \cdot \vec{a}_3|}$$

b) $\vec{b}_1 = 2\pi \dfrac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$

So $\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3) = 2\pi \dfrac{(\vec{a}_2 \times \vec{a}_3) \cdot (\vec{b}_2 \times \vec{b}_3)}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$

Now $(\vec{a}_2 \times \vec{a}_3) \cdot (\vec{b}_2 \times \vec{b}_3)$

$= \varepsilon_{ijk} a_{2j} a_{3k} \varepsilon_{ilm} b_{2l} b_{3m}$

using summation convention and antisymmetric Levi Civita tensor $\varepsilon_{ijk} = \begin{cases} 0 & \text{unless } i,j,k \text{ all different} \\ \pm 1 & \text{depending on whether } ijk \text{ is even } (+) \text{ or odd } (-) \text{ permutation of } 123 \end{cases}$

$(\vec{A} \times \vec{B})_i = \varepsilon_{ijk} A_j B_k$

Use identity $\varepsilon_{ijk} \varepsilon_{ilm} = \delta_{jl} \delta_{km} - \delta_{jm} \delta_{kl}$

$\Rightarrow (\vec{a}_2 \times \vec{a}_3) \cdot (\vec{b}_2 \times \vec{b}_3) = (\delta_{jl} \delta_{km} - \delta_{jm} \delta_{kl}) a_{2j} a_{3k} b_{2l} b_{3m}$

$= a_{2j} b_{2j} a_{3k} b_{3k} - a_{2j} b_{3j} a_{3k} b_{2k}$

$= (\vec{a}_2 \cdot \vec{b}_2)(\vec{a}_3 \cdot \vec{b}_3) - (\vec{a}_2 \cdot \vec{b}_3)(\vec{a}_3 \cdot \vec{b}_2)$

$= (2\pi)(2\pi) - (0)(0)$

So $\boxed{\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3) = \dfrac{(2\pi)^3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = \dfrac{2\pi^3}{v}}$

c) n^{th} BZ is region of k-space that have the origin as their n^{th} nearest neighbor R.L. point.

Let $\{\vec{k}\}$ be the set of points in k-space that have the origin as their n^{th} nearest neighbor R.L. point. Let $\{\vec{k}+\vec{K}\}$ be the set of points $\{\vec{k}\}$ translated by the R.L. $\vec{K}$.
$\Rightarrow \{\vec{k}+\vec{K}\}$ are the set of points that have $\vec{K}$ as their n^{th} nearest neighbor R.L. point.
Consider the sets $\{\vec{k}+\vec{K}\}$ as $\vec{K}$ varies through all R.L. points. Clearly every point $\vec{k}$ in k-space belongs to one of the sets $\{\vec{k}+\vec{K}\}$, since every point $\vec{k}$ has some n^{th} nearest neighbor $\vec{K}$. Also, no point $\vec{k}$ belongs to two different sets $\{\vec{k}+\vec{K}\}$ and $\{\vec{k}+\vec{K}'\}$ since the n^{th} nearest neighbor R.L. point to $\vec{k}$ is unique (unless $\vec{k}$ lies on a Bragg plane in which case it might be on the boundary of the n^{th} BZ - if so we include only half these boundary points in the n^{th} BZ so as not to double count). Since every point belongs in one and only one set $\{\vec{k}+\vec{K}\}$ (except for boundary points of n^{th} BZ), the sets $\{\vec{k}+\vec{K}\}$ cover all k-space with no voids and no overlaps. $\Rightarrow \{\vec{k}\}$ is a primitive cell of the reciprocal lattice.