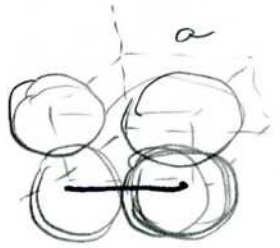
Physics 880.20 Spring 2008

Answers To HW Set #1

1. a) primitive



$V_{cell} = a^3$

$a = 2r$

Each sphere lies at a cube corner & touches 8 cubes.

$V_{spheres} = 8 \times \frac{1}{8}\left(\frac{4}{3}\pi r^3\right)$

$V_s = 4/3\ \pi (a/2)^3 = \pi/6\ a^3$

$V_s = 0.52\, V_{cell}$

b) bcc

(face) center sphere lies totally within cube, while spheres on face touch 8 cubes.

major diagonal $4r = \sqrt{3}\, a$

$V_{cell} = a^3$ $\quad r = \frac{\sqrt{3}\, a}{4}$

$V_s = \frac{4}{3}\pi r^3 + \frac{8}{8}\left(4/3\ \pi r^3\right)$

$= \frac{8}{3}\pi \left\{\frac{\sqrt{3}}{4}\right\}^3 V_{cell}$

$= \frac{\sqrt{3}}{8}\pi\, V_{cell} = 0.68\, V_{cell}$

c) fcc

$V_{cell} = a^3$

(face)

6 faces. Center atom touches 2 cubes.

$4r = \sqrt{2}\, a$

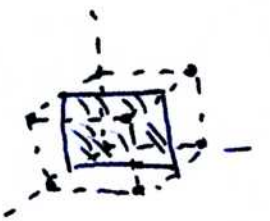
$r = \frac{\sqrt{2}\, a}{4}$

$V_s = 6 \times \frac{1}{2}\left(\frac{4}{3}\pi r^3\right) + \frac{8}{8}\left(\frac{4}{3}\pi r^3\right)$

$V_s = 4\left(4/3\ \pi r^3\right) = 4 \cdot \frac{4}{3} \cdot \frac{2\sqrt{2}\pi a^3}{64}$

$V_s = \frac{\pi\sqrt{2}}{6} V_{cell} = 0.74\, V_{cell}$

2. simple cubic:



(200) Intercepts: $1/2\ \infty\ \infty$