Phy 491
HW#5-Solutions
October 7-14, 2011

5.1

(i) BRAVAIS $\vec{a}_1 = a(1,0,0); \vec{a}_2 = a\left(\frac{1}{2},\frac{1}{2},0\right); \vec{a}_3 = a(0,0,1)$

(ii) NON-BRAVAIS, 3 Atom basis

The primitive lattice vectors are: $\vec{a}_1 = a(1,0,0); \vec{a}_2 = a(0,1,0); \vec{a}_3 = a(0,0,1)$

The basis vectors are: $\vec{r}_1 = a(0,0,0); \vec{r}_2 = a\left(\frac{1}{2},0,\frac{1}{2}\right); \vec{r}_3 = a\left(0,\frac{1}{2},\frac{1}{2}\right)$

(iii) NON-BRAVAIS, 4 Atom basis

The primitive lattice vectors are: $\vec{a}_1 = a(1,0,0); \vec{a}_2 = a(0,1,0); \vec{a}_3 = a(0,0,1)$

The basis vectors are: $\vec{r}_1 = a(0,0,0); \vec{r}_2 = a\left(\frac{1}{2},0,0\right); \vec{r}_3 = a\left(0,\frac{1}{2},0\right); \vec{r}_4 = a\left(0,0,\frac{1}{2}\right)$

5.2

(a) CsCl: Simple Cubic,

n = # of atoms/unit cell volume = $\frac{2}{a^3}$

(b) NaCl: Face Centered Cubic (FCC), $\vec{r}_{Na} = a(0,0,0); \vec{r}_{Cl} = a\left(\frac{1}{2},0,0\right)$

$$n = \frac{2}{a^3/4} = \frac{8}{a^3}$$

(c) CaF_2: Face Centered Cubic (FCC), $\vec{r}_{Ca} = a(0,0,0); \vec{r}_{F1} = a\left(\frac{1}{4},\frac{1}{4},\frac{1}{4}\right); \vec{r}_{F2} = a\left(\frac{3}{4},\frac{3}{4},\frac{3}{4}\right)$

$$n = \frac{3}{a^3/4} = \frac{12}{a^3}$$

(d) $BaTiO_3$; Simple Cubic,

$$\vec{r}_{Ba} = a(0,0,0); \vec{r}_{Ti} = a\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right); \vec{r}_{O1} = a\left(\frac{1}{2},\frac{1}{2},0\right); \vec{r}_{O2} = a\left(0,\frac{1}{2},\frac{1}{2}\right); \vec{r}_{O3} = a\left(\frac{1}{2},0,\frac{1}{2}\right)$$

$$n = \frac{5}{a^3}$$

5.3

$$\vec{b}_2 \bullet \vec{a}_1 = 0 \Rightarrow \vec{b}_1 = \beta\ \hat{y}$$

$$\vec{b}_2 \bullet \vec{a}_2 = 2\pi \Rightarrow \beta\ \hat{y} \bullet \left(a/2\,\hat{x} + a\sqrt{3}/2\,\hat{y}\right) = \beta a\sqrt{3}/2 = 2\pi,\ \beta = \frac{4\pi}{a\sqrt{3}}$$

$$\vec{b}_2 = \frac{4\pi}{a\sqrt{3}}(0,1)$$

$$\vec{b}_1 \bullet \vec{a}_2 = 0 \Rightarrow \vec{b}_1 = \gamma\left(\sqrt{3}/2\,\hat{x} - 1/2\,\hat{y}\right)$$

$$\vec{b}_1 \bullet \vec{a}_1 = 2\pi \Rightarrow \gamma a\sqrt{3}/2 = 2\pi;\ \gamma = \frac{4\pi}{a\sqrt{3}} = \beta$$

$$\vec{b}_1 = \frac{4\pi}{a\sqrt{3}}\left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right)$$

In the reciprocal space the two primitive vectors are $\vec{b}_1$ *and* $\vec{b}_2$ which generate A 2d hexagonal lattice (net) with the sides of the triangle $\beta = \frac{4\pi}{a\sqrt{3}}$

The area of the 1st BZ is the area of the primitive cell in the reciprocal lattice space. This is given by $A_{BZ} = \beta^2 \frac{\sqrt{3}}{2} = \frac{8\pi^2}{a^2\sqrt{3}}$. The area of the primitive cell in the direct lattice space is $A = a^2 \frac{\sqrt{3}}{2}$. Thus we find $A_{BZ} = \frac{(2\pi)^2}{A}$.