Solutions

HW #2.

ECE 606

Q.1 Nearest neighbours for bcc := 8

(For the lattice point 0, 0, 0).

$\left(\pm\frac{1}{2}, \pm\frac{1}{2}, \pm\frac{1}{2}\right)a$

Second nearest neighbour = 6

$(\pm1, 0, 0)a$, $(0, \pm1, 0)a$, $(0, 0, \pm1)a$

FCC:

For the lattice point (0, 0, 0)

Nearest neighbours = 12.

$\left(0, \pm\frac{1}{2}, \pm\frac{1}{2}\right)a$. $\left(\pm\frac{1}{2}, 0, \pm\frac{1}{2}\right)a$ and $\left(\pm\frac{1}{2}, \pm\frac{1}{2}, 0\right)a$

Second nearest neighbour = 6

$(0, \pm1, 0)a$, $(\pm1, 0, 0)a$ and $(0, 0, \pm1)a$.

Si is diamond lattice.

There are 8 silicon atoms in each unit cell.

Fractional coordinates:

Corners.
$$\begin{Bmatrix} 0, & 0, & 0 \\ 0 & a & 0 \\ 0 & a & a \\ 0 & 0 & a \end{Bmatrix} \begin{Bmatrix} a, & 0, & 0 \\ a, & 0, & a \\ a & a & a \\ a & a & 0 \end{Bmatrix}$$

Faces
$$\begin{Bmatrix} a/2 & 0 & a/2 \\ 0 & a/2 & a/2 \\ a/2 & a & a/2 \end{Bmatrix} \begin{Bmatrix} a & a/2 & a/2 \\ a/2 & a/2 & a \\ a/2 & a/2 & 0 \end{Bmatrix}$$

Sub. Lattices
$$\begin{Bmatrix} a/4 & a/4 & 3a/4 \\ 3a/4 & 3a/4 & 3a/4 \\ 3a/4 & a/4 & a/4 \\ a/4 & 3a/4 & a/4 \end{Bmatrix}$$

Q2 To normalize.

a $|\psi|^2 dV = 1$

$\Rightarrow dV = 4\pi r^2 dr \quad \left(dV = \int_0^R r^2 dr \int_0^\pi \sin\theta \, d\theta \int_0^{2\pi} d\phi \right)$

$\therefore \quad 4\pi A^2 \int_0^\infty e^{-2Zr/a} r^2 dr = 4\pi |A|^2 \frac{a^3}{4Z^3}$

$\Rightarrow A = \sqrt{Z^3/\pi a^3}$

b Probability $P(r)\,dr = 4\pi \rho(r) \, r^2 dr$

$\rho(r) \rightarrow |\psi|^2$

$\therefore \quad P = |\psi|^2 4\pi r^2 = \frac{Z^3}{\pi a^3} e^{-2Zr/a} \, 4\pi r^2$

$\frac{dP}{dr} = 0$ for max. probability.

This gives $\quad 2r e^{-2Zr/a} [1 - Zr/a] = 0$

or $\boxed{r = a/Z}$

Q5 Wave-function $= \sqrt{2/a}\ \sin\left(\frac{n\pi x}{a}\right)$

$\langle x \rangle = \quad \langle \psi^* | x | \psi \rangle\, dx$

$\langle p \rangle = \quad \langle \psi^* | p | \psi \rangle\, dx$

Evaluating the integrals

$$\langle x \rangle = 2/a \int_0^a x \sin^2 \frac{\pi x}{a}\, dx = \frac{a}{2}$$

$$\langle p \rangle = \int_0^a \psi^*(x) \left(-i\hbar \frac{\partial}{\partial x}\right) \psi(x)\, dx = 0$$