

**EE550 – SEMICONDUCTOR SCIENCE & TECHNOLOGY**  
**Assignment No. 1 – Due: 26 April 2004 @ 17.00**

**Question 1**

Heisenberg's Uncertainty Principle states that the simultaneous product consisting of the uncertainty of my knowledge of the position of a quantum particle multiplied by the uncertainty in my knowledge of its momentum is bounded, i.e.

$$\Delta x \cdot \Delta p \geq \hbar/2$$

where  $\hbar = h/2\pi$ . In other words, I can never know the exact position of a particle, without driving my uncertainty about its momentum to infinity!

- (a) Suppose that you want to measure the position of an electron to an accuracy of 1 Å. What then is the minimum measurement error in a simultaneous measurement of its speed?
- (b) Suppose that a proton is placed in a narrow box of length 1 cm at 25°C. The kinetic energy of a particle confined in one dimension is approximately  $\frac{1}{2}k_B T$ , where  $k_B$  is Boltzmann's constant. Compute the quantum number  $n$  of a proton in a box at this kinetic energy. Then calculate the energy necessary for this particle to make a transition from your computed value of  $n$  to  $n+1$ . Do you expect quantum mechanical effects to be important in this system.

Proton mass =  $1.6726 \times 10^{-27}$  kg.

Boltzmann's Constant =  $k_B = 1.38062 \times 10^{-23}$  JK<sup>-1</sup>.

Planck's Constant =  $h = 6.62620 \times 10^{-34}$  Js.

1 Å =  $10^{-10}$  m

For a particle in a one-dimensional box of length  $L$ , the quantum wavefunction is given by

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

and the possible energies allowed to the particle are  $E_n = \frac{n^2 h^2}{8mL^2}$ , where  $n$  is an integer.

**Question 2**

- (a) Show that for a simple square lattice (i.e. a two-dimensional lattice) that the kinetic energy of a free electron ( $V(x)=0$ ) at a corner of the 1st Brillouin Zone is higher than that of an electron at the midpoint of a side face of the zone by a factor of two. Recall that for a square lattice the 1st BZ consists of  $-\pi/a < k_x \leq \pi/a$ ,  $-\pi/a < k_y \leq \pi/a$ .
- (b) What is the corresponding factor for a simple cubic lattice (i.e. a three-dimensional lattice)?
- (c) What bearing might the result of (b) have on the conductivity of divalent metals, i.e. metals with two valence electrons?

### Question 3

Consider a solid crystal constructed by bringing together atoms such that there is a single valence electron per unit cell. If the atoms are very far apart, the electron wavefunctions will be localized about each ionic core, extended band states (i.e. energy states which exist throughout the bulk of the material) will not form, and the material will be an insulator. If the atoms are close together, the localized wavefunctions will overlap leading to the formation of band states and non-zero electrical conductivity.

We can estimate the density at which this occurs by recalling that for a free electron gas, the potential for an isolated charge is screened to yield an exponentially decaying potential. In particular, for a singly charged ion in a free electron gas of density  $n$ , the potential energy will be

$$V(r) = -\frac{e^2}{4\pi\epsilon_0 r} \exp[-k_s r]$$

where  $k_s^2 = \frac{3}{(3\pi^2)^{2/3}} \frac{me^2}{\hbar^2 \epsilon_0} n^{1/3}$  and  $\epsilon_0 = 8.85 \times 10^{-12} \text{ Fm}^{-1}$  is the permittivity of free space,  $e = 1.6 \times 10^{-19} \text{ C}$  is the electron charge and  $m = 9.11 \times 10^{-31} \text{ kg}$  is the electron rest mass, and Planck's Constant  $\hbar = 6.62620 \times 10^{-34} \text{ Js}$ .

This potential is called a *screened Coulomb potential* and  $k_s$  is called the *Thomas-Fermi screening length*.

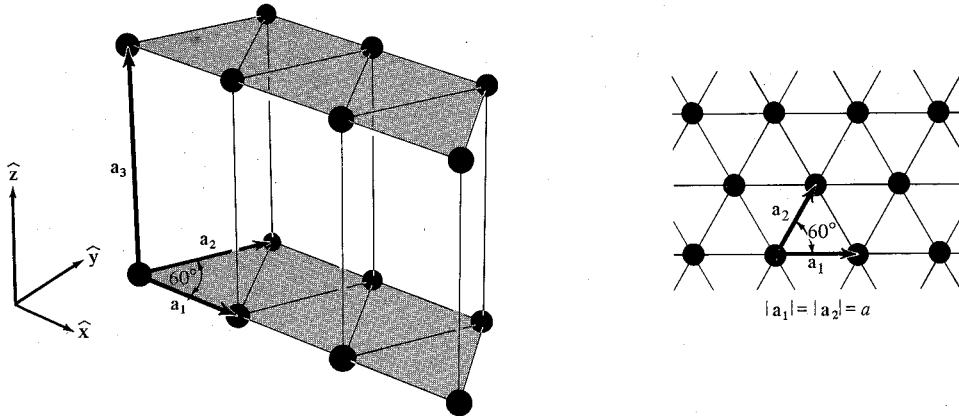
Considering that the lowest bound state of the Coulomb potential given above has a radius given by

$$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{me^2}$$

estimate the density above which the electronic states will not be tightly bound to the ionic cores. Below this density, the atoms are too far apart and the wavefunctions will be highly localized. Above this density, band states will form and the crystal will become a conductor. The transition between these states is called the *Mott transition*.

### Question 4

(Ashcroft & Mermin Ch.5, Q2) Though not a Bravais lattice, the hexagonal close-packed (hcp) structure ranks in importance with the bcc and fcc Bravais lattices; about 30 elements crystallise in the hcp form. Underlying the hcp structure is a simple hexagonal Bravais lattice, given by stacking two-dimensional triangular nets directly above each other:



The simple hexagonal Bravais lattice. Two-dimensional triangular nets (shown in inset) are stacked directly above one another, a distance  $c$  apart.

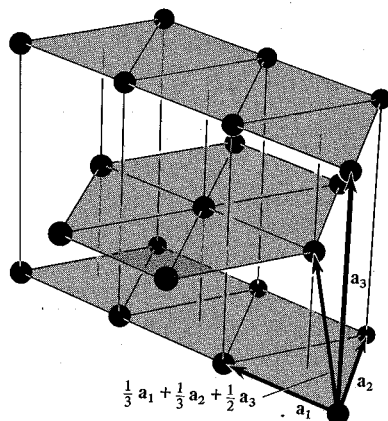
The direction of stacking ( $\mathbf{a}_3$ , above) is known as the  $c$ -axis. The primitive vectors are

$$\bar{\mathbf{a}}_1 = a\hat{x}, \quad \bar{\mathbf{a}}_2 = \frac{a}{2}\hat{x} + \frac{\sqrt{3}a}{2}\hat{y}, \quad \bar{\mathbf{a}}_3 = c\hat{z}$$

[Check these for yourself].

The first two generate a triangular lattice in the  $x$ - $y$  plane, and the third stacks the planes at a distance  $c$  above one another. The hcp structure consists of two interpenetrating simple hexagonal Bravais lattices, displaced horizontally from one another by  $\frac{\bar{\mathbf{a}}_1}{3} + \frac{\bar{\mathbf{a}}_2}{3} + \frac{\bar{\mathbf{a}}_3}{3}$  and

displaced vertically from one another by  $\frac{c}{2}$ , as shown below:



The hexagonal close-packed crystal structure. It can be viewed as two interpenetrating simple hexagonal Bravais lattices, displaced vertically by a distance  $c/2$  along the common  $c$ -axis, and displaced horizontally so that the points of one lie directly above the centers of the triangles formed by the points of the other.

(a) Using the above primitive lattice vectors and the construction

$$\bar{\mathbf{b}}_1 = 2\pi \frac{\bar{\mathbf{a}}_2 \times \bar{\mathbf{a}}_3}{\bar{\mathbf{a}}_1 \cdot (\bar{\mathbf{a}}_2 \times \bar{\mathbf{a}}_3)} \quad \text{etc.}$$

show that the reciprocal of the simple hexagonal Bravais lattice is also simple hexagonal, with lattice constants  $2\pi/c$  and  $4\pi/\sqrt{3}a$ , rotated through  $30^\circ$  about the c-axis with respect to the direct lattice.

(b) For what value of  $c/a$  does the ratio have the same value in both direct and reciprocal lattices?

### Question 5

(Ashcroft & Mermin Ch5, Q4) Prove that any reciprocal lattice vector  $\mathbf{K}$  is an integral multiple of the shortest parallel reciprocal lattice vector  $\mathbf{K}_0$ . *Hint:* Assume the contrary, and deduce that, since the reciprocal lattice is a Bravais lattice, there must be a reciprocal lattice vector parallel to  $\mathbf{K}$  shorter than  $\mathbf{K}_0$ .

### Question 6

We discussed the crystal of silicon in detail. It has the crystal structure of diamond. The basis consists of 8 atoms if the cell is taken as the conventional simple cube.

- (a) What is the structure factor  $S$  of this basis?
- (b) Find the zeros of  $S$  and show that the allowed x-ray reflections of the silicon/diamond structure satisfy  $h+k+l = 4n$ , where all indices are even and  $n$  is any integer, or else all indices are odd.

Remember  $S = \sum_j f_j \exp[i\mathbf{G} \cdot \mathbf{r}_j]$  where  $j$  runs over the  $s$  atoms of the basis,  $f_j$  is the appropriate atomic form factor,  $\mathbf{r}_j$  = positions within the unit cell of the basis atoms and  $\mathbf{G} = h\mathbf{p} + k\mathbf{q} + l\mathbf{r}$ , with  $(hkl)$  = Miller indices.

### Question 7

In the Drude model, as well as in other scattering models, the probability that one electron suffers a collision in a small time interval  $dt$  is  $dt/\tau$ .

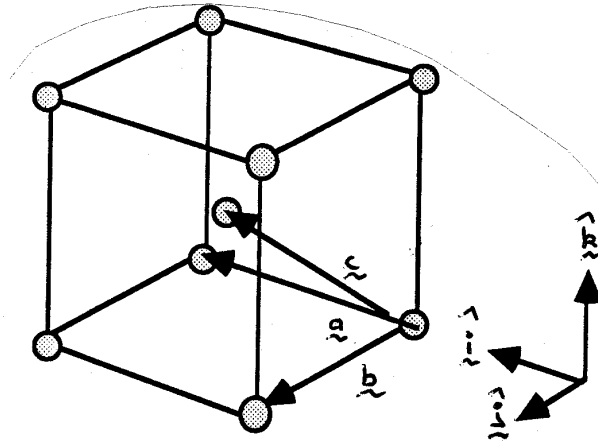
- (a) Show that the probability that an electron picked at time  $t=0$ , will on the average have no collision during the next time  $t$  is given by

$$P(T) = \exp[-t/\tau].$$

- (b) Show that the mean time between two successive collisions is  $\tau$ .
- (c) What is the mobility of electrons in a sample of GaAs where  $\tau$  is calculated to be 1 ps according to the Drude model? Give your results in  $\text{cm}^2\text{V}^{-1}\text{s}^{-1}$ .
- (d) What is the length of a GaAs sample, using the value of  $\tau$  from part (c), that an electron can traverse without scattering with a 90% probability. Assume that there is an electric field of  $10 \text{ kVcm}^{-1}$  and that the electron is injected into the sample with zero velocity.

**Question 8 (ee550 1996)**

Consider the body centred cubic lattice (bcc) shown below:



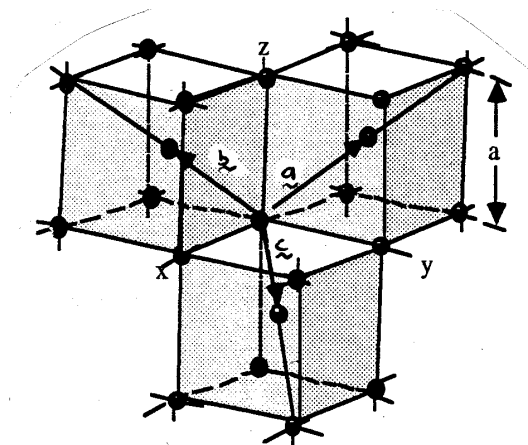
If  $\hat{i}$ ,  $\hat{j}$  and  $\hat{k}$  are three orthogonal unit vectors, then a set of primitive lattice vectors for the bcc lattice could be:

$$\begin{aligned}\vec{a} &= a\hat{i} \\ \vec{b} &= a\hat{j} \\ \vec{c} &= \frac{a}{2}(\hat{i} + \hat{j} + \hat{k})\end{aligned}$$

A more symmetric set for the bcc lattice is:

$$\begin{aligned}\vec{a} &= \frac{a}{2}(\hat{j} + \hat{k} - \hat{i}) \\ \vec{b} &= \frac{a}{2}(\hat{k} + \hat{i} - \hat{j}) \\ \vec{c} &= \frac{a}{2}(\hat{i} + \hat{j} - \hat{k})\end{aligned}$$

as shown below



Calculate the reciprocal lattice of this bcc lattice.

### Question 9

In a simplified model, assume germanium has a single valence band and a single conduction band, with a gap of 0.670 eV. The effective masses are  $m_h = 0.370m_O$  and  $m_e = 0.550m_O$ , respectively, where  $m_O = 9.11 \times 10^{-31}$  kg is the free electron rest mass. We also know that

$$E_{Fi} = \frac{E_C + E_V}{2} + \frac{k_B T}{2} \ln \left[ \frac{N_C}{N_V} \right] \text{ where}$$

$$N_C = 2 \left( \frac{m_e k_B T}{2\pi \hbar^2} \right)^{3/2} \text{ and } N_V = 2 \left( \frac{m_h k_B T}{2\pi \hbar^2} \right)^{3/2}.$$

- Calculate:
- (a) the Fermi energy relative to the top of the valence band
  - (b) the chemical potential (i.e.  $E_{fi} - E_F$ ) at 300 K, relative to the Fermi energy
  - (c) the occupation probability at 300 K for a state at the bottom of the conduction band
  - (d) the probability at 300 K that a state at the top of the valence band is empty
  - (e) the electron concentration in the conduction band at 300 K.

Boltzmann's Constant  $= k_B = 1.38062 \times 10^{-23}$  JK<sup>-1</sup>.

Planck's Constant  $= \hbar = 6.62620 \times 10^{-34}$  Js.

Electron charge  $= e = q = 1.6 \times 10^{-19}$  C.