THE OPEN UNIVERSITY OF SRI LANKA

DEPARTMENT OF PHYSICS

BACHELOR OF SCIENCE DEGREE PROGRAMME -2011/2012 -LEVEL 05

PYU 3173 – SOLID STATE PHYSICS   Final Examination – 2011/2012

TIME: TWO HOURS (2 hrs)   ANSWER FOUR QUESTIONS ONLY

Date : 17th December 2011   Time : 1.00 pm to 3.30 pm

You may assume that, mass of electron $m_e = 9.1 \times 10^{-31}$ kg, $h = 6.63 \times 10^{-34}$ J s, $\pi = 3.14$, $\hbar = 1.05 \times 10^{-34}$ J s, $c = 3 \times 10^8$ m s^{-1}, 1 eV = 1.6×10^{-19} J.

1) Define the terms Bravais lattice, primitive unit cell, conventional unit cell, lattice constant and basis.

   Identify the Bravais lattice and basis that would generate the hexagonal close packed (*hcp*) structure.

   Show that the c/a ratio of the unit cell dimensions of an *hcp* lattice is $\sqrt{8/3}$.

   Zinc has an *hcp* structure with lattice parameters a and c as 2.66 Å and 4.95 Å respectively. If the atomic radius and the atomic mass of zinc are 1.31 Å and 65.37 *amu* respectively, find the packing fraction and density of zinc.

2) Show that for any cubic lattice the separation of the planes corresponding to Miller indices (*hkl*) is given by:

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

   Where a is the lattice parameter.

   Briefly describe the Bragg's diffraction in crystals and show that the Bragg condition for crystal diffraction on (*hkl*) planes is given by:

$$2d_{hkl} sin\theta_{hkl} = n\lambda,$$

   Where the symbols have their usual meanings.

   Determine the Bragg angles for the (111), (220), (311), and (400) reflections of Germanium which has a cubic structure with lattice parameter 5.65 A° using "Copper K_α" X-rays which has a wavelength $\lambda = 0.154$ nm.

3) The potential energy of two atoms in a diatomic molecule is approximated by

$$U(r) = \frac{a}{r^{12}} - \frac{b}{r^{6}}$$

where r is the spacing between the molecules and a and b are positive constants.

(a) Show that the force $F(r)$ on one atom because of the other is given by

$$F(r) = \frac{12a}{r^{13}} - \frac{6b}{r^{7}}$$

(b) Show that the atoms are in equilibrium (sit at rest with respect to each other) if

$$r = \left[\frac{2a}{b}\right]^{\frac{1}{6}}$$

(c) With the aid of a sketch of both $U(r)$ and $F(r)$, comment on whether this equilibrium is stable or unstable.

(d) Show .that the minimum energy required to dissociate the molecule – that is, to separate the two atoms to an infinite distance apart, is

$$E = \frac{b^2}{4a}$$

(e) For the molecule CO, the equilibrium distance between the carbon and oxygen atoms is 1.13×10^{-10} m and the dissociation energy is 1.54×10^{-18} J per molecule. Find the values of the constants a and b.

4) A simple, one dimensional model of a solid consists of a series of masses, each of mass m, joined by springs of spring constant K, with an equilibrium separation of a.

(a) Write down an equation of motion for the nth atom in terms of the displacement of the $n-1$, n and $n+1$ atoms.

(b) Show that the relation between the frequency ω and wave-vector k (the dispersion relation) is

$$\omega^2 = 4\frac{K}{m}\sin^2\left(\frac{ka}{2}\right)$$

(c) Using the result obtained in part (b), show that in a simple one dimensional of a solid consists of a series of masses, each of mass m, joined by springs of spring constant K, with an equilibrium separation of a, the dispersion curve meets the zone boundary normally.

5) (a) By considering the volume of a spherical shell in 'k-space' and the volume occupied by each electron state, show that the free electron density of states is given by

$$g(E)=\frac{V}{2\pi^2\hbar^3}(2m_e)^{\frac{3}{2}}E^{\frac{1}{2}}$$

(b) The average energy of a free electron can be written as

$$\langle E\rangle=\frac{1}{N}\int_0^{E_F}E\,g(E)\,dE$$

where N is the total number of free electrons. Show that (at 0 K) the average energy of an electron in a metal is 60% of the Fermi energy (E_F).

(c) Silver has 1 free electron per atom and a face centred cubic structure with conventional unit cell length, a= 0.409 nm. Calculate the Fermi energy of silver at absolute zero. Hence determine the average energy of a free electron in Silver at absolute zero.

Assume that the Fermi energy at absolute zero as $E_F=\frac{\hbar^2}{2m_e}\left(\frac{3\pi^2 N}{V}\right)^{\frac{2}{3}}$ and the symbols have their usual meanings.

6) An electron with energy E is incident on a potential step with height $U_0 > E$. The situation may be described by the 1-D time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+U(x)\psi(x)=E\psi(x)$$

with potential: $$U(x)=\begin{cases}0 & \text{for } x<0\\ U_0 & \text{for } x\geq 0\end{cases}$$

(a) If the wave function in the region x < 0 is, $\psi_1(x)=Pe^{ikx}+Qe^{-ikx}$, using the Schrödinger equation, determine the value of k.

(b) If the wave function in the region $x\geq 0$ is $\psi_2(x)=Re^{-i\alpha x}$, using the Schrödinger equation, determine the value of α.

(c) State the boundary conditions which should be imposed on the wave function described in part (a) and part (b).

(d) Why are these boundary conditions necessary?

(e) Using the boundary conditions on the wave function that you have mentioned in part (b), show that

$$\frac{P}{Q}=\frac{k+i\alpha}{k-i\alpha}$$

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