National University of Singapore

PC3235 Solid State Physics I

(Semester I: AY2009-10, 25 November)

Time Allowed: Two Hours

INSTRUCTIONS TO CANDIDATES

1. This examination paper contains **FOUR** questions and comprises **FIVE** printed pages.
2. Answer any **THREE** questions.
3. Answers to the questions are to be written in the answer books.
4. This is a CLOSED BOOK examination.
5. A Table of Constants is provided.

1. Barium possesses a bcc structured space lattice. It belongs to group II in the periodic table. Given that:

lattice constant $a = 5.02A$; density $= 3.51 g/cm^3$; molar mass $= 137.33 gmol^{-1}$;

electrical resistivity at $300K = 332n\Omega \cdot m$; mass of electron $= 9.1\times10^{-31} kg$;

$\hbar = 1.054\times10^{-34} Js$; Avogadro's number $= 6.02\times10^{23} atom/mol$;

$e = 1.60\times10^{-19} Coulomb$

(a) Calculate the concentration of the conduction electrons.

[5 marks]

(b) Calculate the mean free path. Assume that electrons follow the free electron model.

[5 marks]

(c) Calculate the Fermi Energy.

[5 marks]

(d) Sketch two possible band structures to explain how barium behaves as a metal.

[5 marks]

(e) The conventional unit cube of a bcc structure contains two atoms. Find the structure factor S of this basis and obtain the allowed reflections of the bcc structure.

[3 marks, 2 marks]

2. (a) Assume that the density of orbitals, $D(E)=n_o$ where n_o is a constant in unit of $\left(cm^3eV\right)^{-1}$. Show that the expression for the electron concentration, n in the conduction band of an intrinsic semiconductor is

$$n = n_o k_B T e^{-(E_c - E_F)/k_B T}$$

where E_c is the energy at the conduction band edge and E_F is the Fermi level. State and justify clearly the assumption you have made in the derivation.

[7 marks]

(b) Derive a corresponding expression for the concentration of holes (p) in the valence band.

[6 marks]

(c) From the definition of the intrinsic Fermi level(E_F), find the location of E_F in relation to E_c and E_v where E_v is the energy at the valence band edge.

[6 marks]

(d) Calculate the electron concentration (n) at room temperature $\left(k_B T = \frac{1}{40} eV\right)$ for a semiconductor with $E_g = 1.5eV$ and $n_o = 2\times10^{21}\left(cm^3 \cdot eV\right)^{-1}$.

[6 marks]

3. (a) Consider a NaCl structure ionic crystal with a repulsive potential energy b/r^n between nearest neighbors. Write the total energy (U) of a system of $2N$ ions of alternating charge $\pm q$ in terms of nearest neighbor distance r, Madelung constant α and parameters b and n. Also discuss briefly how parameters b and n can be determined from the experimental data.

[8 marks]

(b) Sketch a phonon dispersion for a NaCl crystal. Discuss their behavior at zone centre and zone boundary.

[5 marks]

(c) Compare the dispersion relation behavior at the zone centre and the zone boundary of Si with that of NaCl crystal.

[4 marks]

(d) Derive an expression for Debye density of state for a one-dimensional linear chain of length Na with lattice constant a, atomic mass M, and interatomic force constant C. Also determine the Debye cut off frequency. The dispersion relation of the system is

$$\omega = 2\sqrt{\frac{C}{M}}\left|\sin\frac{1}{2}ka\right|$$

[8 marks]

4. (a) Discuss the periodicity of (i) Bloch function in real space and (ii) Bloch function and eigen-energy in the reciprocal space in energy band theory.

[6 marks]

(b) Show that the density of orbitals, $D(E_F)$ at the Fermi energy (E_F) for 3-D free electron is

$$D(E_F)=\frac{V}{2\pi^2}\frac{k_F^3}{E_F}$$

[6 marks]

(c) Given that the primitive vectors of the fcc Bravais lattice are

$$\vec{a}_1=\frac{a}{2}(0,1,1);$$

$$\vec{a}_2=\frac{a}{2}(1,0,1);$$

$$\vec{a}_3=\frac{a}{2}(1,1,0);$$

show that the reciprocal vectors $\vec{b}_1$, $\vec{b}_2$ and $\vec{b}_3$ of fcc Bravais lattice are:

$$\vec{b}_1=\frac{2\pi}{a}(\bar{1},1,1)$$

$$\vec{b}_2=\frac{2\pi}{a}(1,\bar{1},1)$$

$$\vec{b}_3=\frac{2\pi}{a}(1,1,\bar{1})$$

[6 marks]

(d) Calculate and sketch the two lowest free electron energy levels for the fcc Bravais lattice. The (h,k,l) values of the two lowest energy levels are $(0,0,0)$ and $(0,\bar{1},\bar{1})$ accordingly. The energies are to be plotted along $\Gamma(k=0)$ to $H\left(k=\frac{2\pi}{a}\hat{x}\right)$ line.

[7 marks]

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