

UNIVERSITY COLLEGE LONDON

EXAMINATION FOR INTERNAL STUDENTS

MODULE CODE : PHAS3225

ASSESSMENT : PHAS3225A
PATTERN

MODULE NAME : Solid State Physics

DATE : 30-Apr-15

TIME : 10:00

TIME ALLOWED : 2 Hours 30 Minutes

Answer EVERY question from section A and TWO questions from section B.

The numbers in square brackets in the right-hand margin indicate the provisional allocation of maximum marks per sub-section of a question.

Mass of the electron	m_e	=	$9.11 \times 10^{-31} \text{ kg}$
Charge on the electron	e	=	$-1.602 \times 10^{-19} \text{ C}$
Permittivity of free space	ϵ_0	=	$8.854 \times 10^{-12} \text{ F m}^{-1}$
Boltzmann's constant	k_B	=	$1.38 \times 10^{-23} \text{ J K}^{-1}$
Planck's constant/ 2π	\hbar	=	$1.05 \times 10^{-34} \text{ J s}$
Speed of light	c	=	$3 \times 10^8 \text{ m s}^{-1}$

SECTION A

[Part marks]

1. A two-dimensional solid forms a crystal structure with a rectangular unit cell, a basis composed of atoms of type A and B with fractional coordinates of (0,0) and (1/2,1/2), respectively, and lattice vectors $\mathbf{a}_1=(a,0)$ and $\mathbf{a}_2=(0,b)$.

Make a sketch of the structure spanning several unit cells.

[2]

Assuming that $b=\sqrt{2}a$, show that to avoid like atoms touching their radii must obey the inequality $r_B/r_A > \sqrt{3} - 1$.

[4]

2. KCl is an example of an ionically bonded crystal for which the cohesive energy per ion pair may be written as

$$U(r) = A \exp(-r/\rho) - \frac{\alpha Z^2}{4\pi\epsilon_0 r},$$

where r is the nearest neighbour distance, Z is the ionic charge.

Explain the origins of the two terms and the meaning of the symbols A , ρ and α .

[3]

For a crystal of KCl, calculate the cohesive energy per ion pair relative to the separated neutral gas atoms, expressing your answer in units of eV.

[4]

(For KCl, $A=2.05 \times 10^{-15} \text{ J}$, $\rho=0.326 \text{ \AA}$, $r=3.147 \text{ \AA}$, $\alpha=1.748$; K has a first electron ionisation energy of 4.34 eV, Cl an electron affinity of 3.61 eV.)

3. The dispersion relation of longitudinal phonons propagating along a one dimensional chain of atoms is given by

$$\omega = \sqrt{\frac{4C}{M}} |\sin(ka/2)|,$$

where ω is the frequency of vibration, k is the phonon wavevector, C is the force constant, a is the equilibrium spacing between the atoms, and M is the atomic mass.

Make a sketch of the dispersion relation, being careful to label the axes appropriately. Identify the location of the Brillouin zone boundary. [2]

Derive an expression for the *group velocity* from the phonon dispersion relation. Give a physical explanation for the value of the phonon group velocity at the Brillouin zone boundary. [4]

4. For semiconductors, explain what is meant by the terms *direct band gap* and *indirect band gap* by making reference to the electronic band structure in each case. Illustrate your answer with appropriately annotated sketches of the band structure in each case. [4]

For a semiconductor with an indirect band gap, make a sketch of the energy dependence of the photon absorption coefficient. Relate any energy scales to those shown in the sketch of the band structure, and indicate regions of transparency and opacity. [3]

5. Write down the general form of the reciprocal lattice vectors \mathbf{G} of the simple cubic lattice in terms of the Miller indices (h, k, l) . [2]

By constructing the scattering triangle derive an expression for the modulus of the wave vector transfer Q relevant for elastic scattering in terms of the X-ray wavelength λ and Bragg angle θ . [2]

State the Laue condition and use it to derive an expression for λ as a function of the other variables in the problem. By comparing it with Bragg's law, deduce an expression for the plane spacing d as a function of a and (h, k, l) . [3]

6. In tight-binding theory, the electron energy E_k as a function of wave vector k may be written as

$$E_k = -\alpha - \gamma \sum_m \exp(-ik \cdot \mathbf{r}_m),$$

where the sum is over nearest neighbours connected by the vector \mathbf{r}_m . Write down the typical form of the integrals α and γ . [4]

Evaluate E_k for a (two-dimensional) square lattice of atoms spaced a apart as a function of wavevector components k_x and k_y pointing parallel to the two edges of the square. [3]

SECTION B

7. This question is about using X-rays to determine the structure of an unidentified element which is known to have either the body centred cubic (BCC) or face centred cubic (FCC) structure.
- (a) By adopting a conventional cubic unit cell, describe using annotated figures how the BCC and FCC structures can be decomposed into a simple cubic lattice and a basis. In each case, identify the basis atoms and write down their coordinates. [6]
- (b) Write down the general expression for the X-ray unit cell structure factor being careful to define any terms that you introduce. [3]
- (c) Obtain expressions for the unit cell structure factor of the BCC and FCC structures using the conventional unit cell and deduce the restriction on values of (hkl) for the observation of diffraction peaks. [6]
- (d) In an X-ray scattering experiment using a monochromatic beam of wavelength 1.5 \AA on a powdered sample of the unknown element, the first three Bragg peaks are observed at scattering angles $2\theta = 27.27, 38.94$ and 48.19° . Using these data, assign Miller indices to these reflections and hence deduce whether the material adopts either the BCC or FCC structures, and calculate its lattice constant. [8]
- (e) Using your answer to part (c), in conjunction with annotated figures, identify the reciprocal space lattices of the BCC and FCC real space lattices, being careful to label the figures appropriately. Validate your answer for the FCC real space lattice by the explicit calculation of its reciprocal primitive lattice vectors. [7]

8. This question relates to the carrier concentrations in semiconductors.

(a) Explain what is meant by the terms *intrinsic* and *extrinsic* semiconductors. With the aid of suitably annotated diagrams, distinguish between the cases of *n*- and *p*-type extrinsic semiconductors, indicating the states that give rise to extrinsic behaviour in both cases. Take care to define any terms you use. [6]

(b) The density of electron states $g(\mathcal{E})$ in the conduction band of a semiconductor with an energy gap \mathcal{E}_G is given by

$$g(\mathcal{E}) = \frac{V}{2\pi^2\hbar^3} (2m_e^*)^{3/2} (\mathcal{E} - \mathcal{E}_G)^{1/2},$$

where m_e^* is the effective mass of the electron, V is the volume of the crystal and the zero of energy is equal to the top of the valence band. Show that the intrinsic number of electrons per unit volume in the conduction band is given by

$$n_i = N_C e^{(\mu - \mathcal{E}_G)/k_B T},$$

where N_C is a temperature dependent constant which you should determine, and μ is the chemical potential. (Note: $\int_0^\infty x^{1/2} e^{-x} dx = \sqrt{\pi}/2$.) [8]

(c) Find the corresponding expression for the intrinsic number of holes p_i per unit volume in the valence band. Hence derive the law of mass action for the electron and hole concentrations valid for any semiconductor. [8]

(d) Now consider an extrinsic semiconductor with acceptor and donor concentrations of N_A and N_D , respectively. Starting from the equation for charge neutrality, and assuming all dopants are fully ionised, show that the concentration n of electrons in the conduction band is given by

$$n = \frac{1}{2} \left(\sqrt{\Delta^2 + 4I^2} + \Delta \right)$$

where $\Delta = N_D^+ - N_A^- > 0$ is the doping, and I is the intrinsic carrier density. Find the limiting forms of n in either the extrinsic ($\Delta \gg I$) or intrinsic limits ($I \gg \Delta$). [8]

9. This question is about the lattice vibrations (phonons) and specific heat of a one-dimensional (1D) chain of N atoms.

(a) Assuming periodic boundary conditions, show that in 1D the density of states with respect to frequency ω is given in general by

$$g(\omega) = \frac{L}{\pi} \frac{dk}{d\omega},$$

where k is the modulus of the phonon wavevector and L is the length of the chain. [3]

(b) Hence show that the density of states is given by

$$g(\omega) = \frac{2N}{\pi\omega_{ZB} (1 - \omega^2/\omega_{ZB}^2)^{1/2}},$$

where ω_{ZB} is the frequency at the Brillouin zone boundary. Make a sketch of $g(\omega)$ versus ω and comment on the result. (The 1D form of the phonon dispersion is given by

$$\omega = \sqrt{\frac{4C}{M}} |\sin(ka/2)|,$$

where ω is the frequency of vibration, k is the phonon wavevector, C is the force constant, a is the equilibrium spacing between the atoms, and M is the atomic mass.) [6]

(c) State the key assumptions used in the Debye theory of the specific heat of insulating solids. [3]

(d) Show using Debye theory that the specific heat of the 1D chain at a temperature T may be written as

$$C_V = \frac{Nk_B T}{\Theta_D} \int_0^{\Theta_D/T} \frac{x^2 e^x}{(e^x - 1)^2} dx,$$

where Θ_D is the Debye temperature and $x = \hbar\omega/k_B T$. [11]

(e) Determine the dependence of C_V on T in the high and low temperature limits. Comment on your answers with reference to classical theory and the predictions of Debye theory for a three-dimensional solid. (Note: $\int_0^\infty x^2 e^x / (e^x - 1)^2 dx = \pi^2/3$.) [7]

10. This question is about the formation of electronic energy bands in crystalline solids using the nearly free electron model.

Start by considering a one-dimensional material formed from a chain of N atoms separated by a distance a and of overall length L .

- (a) Sketch the free-electron energy dispersion relation, identify the position of the Brillouin zone (BZ) boundaries, and indicate the positions of the Fermi Level assuming that the atoms are i) monovalent and ii) divalent. [4]

Now take into consideration the fact that the electrons interact with the periodic potential $V(x)$ from the positively charged ion cores.

- (b) Discuss in detail what happens when the electron's wavevector lies on the BZ boundary. [5]

- (c) Justify why the electronic wavefunction at the BZ boundary can be written as

$$\psi^\pm(x) = \frac{1}{\sqrt{2L}} (\exp(i\pi x/a) \pm \exp(-i\pi x/a)).$$

Discuss what the two forms represent both in terms of the spatial distribution of electronic charge and the consequences for the band structure in the vicinity of the BZ boundary. [5]

- (d) Assuming that the periodic potential is given by

$$V(x) = -V_1 \cos\left(\frac{2\pi x}{a}\right),$$

use first-order perturbation theory to calculate the energy difference between the two forms of $\psi^\pm(x)$. Hence sketch the nearly-free electron theory dispersion in one dimension, and explain how this allows us to understand why some materials are metals while others form insulators. [8]

- (e) For a two dimensional material with a square lattice, describe with the aid of appropriately labelled figures how the Fermi surface in the nearly-free electron theory evolves as the valence of the atoms is increased from one to two. [8]