UNIVERSITY COLLEGE LONDON

EXAMINATION FOR INTERNAL STUDENTS

MODULE CODE : **PHAS3225**

ASSESSMENT PATTERN : **PHAS3225A**

MODULE NAME : **Solid State Physics**

DATE : **12-May-14**

TIME : **10:00**

TIME ALLOWED : **2 Hours 30 Minutes**

TURN OVER

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

SECTION A

[Part marks]

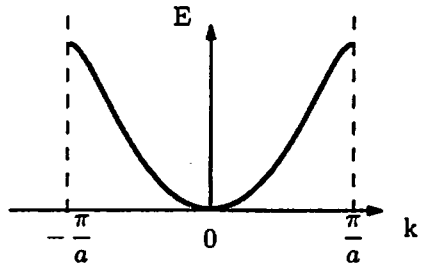
1. For an ionic solid, such as NaCl, the cohesive energy per ion pair may be written as

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

where r is the nearest neighbour distance, Z is the ionic charge, ρ is a material dependent length scale, and α=1.748. Explain briefly the origins of the two terms. [2]
Show for this solid that $A = \alpha Z^2 \rho \exp(r_0/\rho)/(4\pi\epsilon_0 r_0^2)$, where r_0 is the equilibrium nearest-neighbour distance. [4]

2. Using the conventional unit cell draw cross-sections through the body centred cubic (*bcc*) structure perpendicular to the [001] direction for z=0, $a/2$ and a, where a is the cubic unit cell parameter and z is the fractional coordinate in the [001] direction. [3]
Calculate the maximum packing fraction of spheres in an ideal *bcc* solid. [3]

3. Write down the expression for the kinetic energy E of a free electron of wavevector k, and show how the electron mass can be written in terms of a derivative of E. [3]
Shown below is a typical energy band calculated using the nearly free electron model.



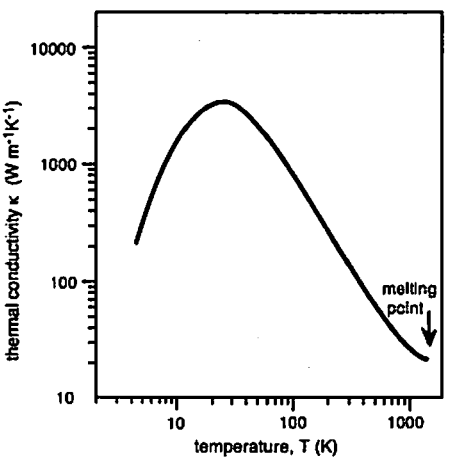
Explain what is meant by the term *effective electron mass* and describe using a sketch how it varies for the band shown above as a function of k. [4]

4. The electron and hole densities for a particular semiconductor may be written respectively as

$$n = A\,(m_e^* T)^{3/2}\, e^{(\mu - E_G)/k_B T},$$
$$p = A\,(m_h^* T)^{3/2}\, e^{-\mu/k_B T},$$

where A is a constant, E_G is the band gap, and other symbols have their usual meaning.
For an intrinsic semiconductor, derive an expression for the temperature dependence of the chemical potential μ. [3]
Sketch the band structure of a typical intrinsic semiconductor, label the conduction and valence bands, the band gap and indicate the position of the chemical potential. [4]

5. The figure below shows the thermal conductivity κ of a sample of silicon.



The thermal conductivity may be written as the product of three physical quantities. What are they? [3]
Describe what is meant by the terms *normal* and *Umklapp* phonon scattering and describe how these concepts may be used to understand the temperature dependence of κ shown in the figure. [4]

6. State Bragg's law for the constructive interference of X-rays of wavelength λ scattered through an angle 2θ by lattice planes of spacing d in a crystal. [1]
Show that for a cubic system the Miller indices (h, k, l) of all allowed Bragg reflections must satisfy the inequality

$$(h^2 + k^2 + l^2) \leq \frac{4a^2}{\lambda^2},$$

where a is the lattice constant. [3]
Determine the Miller indices of the highest angle Bragg reflection that can be observed with a=0.3 nm and λ=0.34 nm. [3]

SECTION B

7. In this question you are asked to consider the phonon contribution to the specific heat of a two dimensional monatomic crystal.

(a) Explain why in two dimensions the classical value of the specific heat is expected to be $C_V = 2Nk_B$ where N is the number of atoms. [3]

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

(c) Show that for the two dimensional monatomic crystal, the density of phonon states as a function of frequency ω is given by

$$g(\omega) = \frac{2N}{\omega_D^2}\omega,$$

where ω_D is the Debye Frequency. [5]

(d) Explain why according to Debye theory the internal energy U of the two dimensional crystal may be written as

$$U = U_z + \frac{4N}{\omega_D^2}\int_0^{\omega_D} \frac{\hbar\omega^2}{\exp(\hbar\omega/k_BT) - 1} d\omega,$$

where U_z is a constant. [4]

(e) From the expression for U given above deduce an expression for C_V, and determine its limiting behaviour at low temperatures. Comment on the result with reference to the behaviour expected for a three dimensional system. [9]

(f) Confirm by explicit calculation that C_V approaches its classical value in the limit of high temperature. [6]

(Note: $\int_0^\infty x^3 e^x/(e^x - 1)^2 dx \approx 7.21$.)

8. This question is about X-ray scattering from copper, which crystallises in the face centred cubic (*fcc*) structure, and the different structures that are formed when it is alloyed with other elements.

(a) Write down the general expression for the unit cell structure factor and state the general condition for it to be non zero. Ensure that you define any terms that you introduce. [5]

(b) Using the conventional cubic cell identify the lattice and the basis needed to generate the *fcc* structure making use of annotated sketches where necessary. [4]

(c) Derive an expression for the *fcc* unit cell structure factor. Determine the condition on the Miller indices (h, k, l) for the Bragg reflections to have non-zero intensity. List as a function of increasing scattering angle the Miller indices of the first three unique reflections observable in a powder diffraction experiment. [5]

(d) A diffraction experiment is performed on copper using radiation with a wavelength of λ=0.150 nm. The first three Bragg reflections are recorded at scattering angles 2θ of 42.18, 49.10, and 71.97 degrees. Using this data assign Miller indices to these reflections and deduce the lattice parameter a of copper. [9]

(e) β-brass is a binary alloy consisting of equal numbers of copper and zinc atoms which sit on the sites of a body centred cubic (*bcc*) lattice. At temperatures above the critical temperature of T_C=733 K, each lattice site is randomly occupied by either a copper or a zinc atom. On cooling below T_C, β-brass forms the ordered CsCl structure with, say, the copper atoms occupying the body centres and the zinc atoms the vertices of the conventional *bcc* unit cell. By explicit evaluation of the unit cell structure factor above and below T_C describe how the transition at T_C might be detected in an X-ray scattering experiment. (Hint: above T_C assume that each site of the *bcc* lattice has the average scattering power of copper and zinc.) [7]

9. This is a question about the $p-n$ semiconducting junction.

(a) Define what is meant by the terms p-type and n-type doped semiconductors. Draw energy level diagrams for samples of p and n doped semiconductors, and identify the position of the energy levels of the dopants in each case. [4]

(b) Describe with the aid of sketches the variation of the energy levels across a $p-n$ junction, and the variation of free carrier density, $\rho(x)$. Explain where in your sketch the "depletion zone" is located. [6]

(c) Given that the potential $\Phi_0(x)$ across the junction obeys Poisson's equation (i.e. $\partial^2\Phi_0(x)/\partial x^2 = -\rho(x)/(\epsilon\epsilon_0)$), use appropriate boundary conditions to show that it may be written as

$$\Phi_0(x) = \begin{cases} \frac{eN_A}{2\epsilon\epsilon_0}(x+w_p)^2 & \text{for } -w_p < x < 0 \\ \Delta\Phi_0 - \frac{eN_D}{2\epsilon\epsilon_0}(x-w_n)^2 & \text{for } 0 < x < w_n. \end{cases}$$

Here N_A (N_D) is the number of acceptor (donor) atoms per unit volume, and w_p (w_n) is the width of the depletion zone on the p (n) side of the junction. [12]

(d) What is the condition for overall electrical neutrality of the junction? Use this condition and the above result for Φ_0 to show that

$$w_n = \left(\frac{2\epsilon\epsilon_0 N_A \Delta\Phi_0}{eN_D(N_A+N_D)}\right)^{1/2}$$

and deduce an analogous expression for w_p. [8]

10. This is a question about a two dimensional metal with a square lattice of spacing a for which the electrons may initially be considered to be free.

(a) State the general expression for a reciprocal lattice vector of the two dimensional square lattice in terms of a. Draw a sketch of the reciprocal lattice, and identify the area of the first Brillouin zone. [5]

(b) For the case that the metal is monovalent, calculate the magnitude of the Fermi wavevector k_F as a fraction of the shortest distance from the origin to the nearest Brillouin zone boundary, and make a sketch of the Fermi surface within the first Brillouin zone. [5]

(c) It is now assumed that the metal is divalent, and that the electrons are affected by the periodic potential of the ion cores. Discuss with the aid of sketches how the shape of the Fermi surface evolves as the strength of the periodic potential is increased from zero. [7]

(d) Derive an expression for the density of states $g(E)$ in energy of the free electron gas in two dimensions, and hence obtain an expression for the Fermi energy E_F as a function of n, the number of electrons per unit area. [7]

(e) At finite temperature the total number of electrons N is given by

$$N = \int_0^\infty g(E) f(E)\, dE$$

where $f(E)$ is the Fermi-Dirac distribution. Evaluate this integral for the two dimensional free electron gas, and use the result to show that the chemical potential $\mu(T)$ at finite temperatures is given by the expression [6]

$$\mu(T) = k_B T \ln\left[\exp(E_F/k_B T) - 1\right].$$

(Hint: $\int_{-c}^{\infty} 1/(\exp(x) + 1) dx = \ln(1 + \exp(c))$.)

END OF PAPER