UNIVERSITY OF SWAZILAND.

FACULTY OF SCIENCE.

DEPARTMENT OF PHYSICS.

MAIN EXAMINATION 2005.

TITLE OF PAPER: SOLID STATE PHYSICS.

COURSE NUMBER: P412.

TIME ALLOWED : THREE HOURS.

ANSWER ANY FOUR QUESTIONS . ALL CARRY EQUAL MARKS.

THIS PAPER IS NOT TO BE OPENED UNTIL PERMISSION HAS BEEN GIVEN BY THE INVIGILATOR.

Question One.

(a) (i) Draw conventional unit cells of face centred and body centred cubic lattices of lattice constant 'a'. For each lattice, write down the number of lattice points per cell and the volume of the primitive cell.

(5 marks)

(ii) Obtain Miller indices of a plane that cuts the crystal axes at points (4,0,0); (0,2,0) and (0,0,3). Calculate the spacing between two such consecutive planes given that its lattice constant is 2.5 Å

(4 marks)

(iii) The molecular weight of NaCl is 58.46. Its density is 2.167 g cm^{-3}. Calculate its lattice constant. (4 marks)

(iv) The planes of a tetrahedron are $(111), (\bar{1}1\bar{1}), (1\bar{1}\bar{1}) and (\bar{1}\bar{1}1)$, Calculate the bonding angle. (4 marks)

(b) (i) Calculate the Bragg angle for second order reflection from (100) planes when 1.54 Å x-rays are incident on a cubic crystal lattice with lattice constant 4.0 Å. Calculate the energy in eV of these x-rays. (3 marks)

(ii) Show that the volume of the first Brillouin zone of a lattice is $(2\pi)^3 / V_c$ where V_c is the volume of the primitive cell in a direct lattice.

(5 marks)

Question Two.

(a) (i) Explain ***ionic bonding*** in crystalline materials. (3 marks)

(ii) What is meant by the phrase ***Madelung energy of ionic crystals***? (3 marks)

(b) Derive an expression for the total lattice energy of a crystal having 2N ions at their equilibrium separation 'R_o'. (12 marks)

(c) A line of 2N ions of alternating charges (+/-) q have a repulsive potential energy of the form A/R^n, between nearest neighbours. Show that at equilibrium separation the potential energy,

$$U_{tot} = \frac{-2Nq^2 \ln 2}{R_0}\left(1 - \frac{1}{n}\right).$$

[Given: Madelung constant = 2 ln2] (7 marks)

Question Three.

(a) State the basic assumptions of Einstein's theory of the specific heat of solids. (3 marks)

(b) Deduce an expression for the heat capacity of solids according to Einstein's theory.

[Given: the mean energy of a harmonic oscillator, $\bar{\varepsilon} = \hbar\omega\left(\frac{1}{2} + \frac{1}{e^{\hbar\omega/kT} - 1}\right)$]

(8 marks)

(c) Show that in the high temperature limit (i.e. $T \gg \hbar\omega/k$) , Einstein's theory agrees with the classical Dulong-Petit law.

[Given that: for small values of x, $e^x \approx 1 + \frac{x}{1!} + \frac{x^2}{2!}$]

(7 marks)

(d) State how, at low temperatures, the specific heat of a solid varies with temperature and discuss how far Einstein's theory agrees with it. (7 marks)

Question Four.

(a) Write down the Laue condition for x-ray diffraction in a crystal. (2 marks)

(b) Show that the above condition is equivalent to Bragg's law given as: $2d \sin \theta = n\lambda$.

(8 marks)

(c) The Geometric structure factor of a crystal is given as:

$$S_G = \sum_{j=1}^{s} f_j \exp\left[-i2\pi(n_{1_j}h + n_{2_j}k + n_{3_j}l)\right],$$ where symbols have their usual meanings. 's 'is the number of atoms of the basis and 'f ' is the atomic form factor.

Explain the significance of this equation with regard to x-ray diffraction in crystals, giving either a b.c.c. or an f.c.c. lattice as a specific example. (10 marks)

(d) In the x-ray photograph of a cubic lattice, lines are observed at the following Bragg angles in degrees:
12.3, 14.1, 20.2, 24.0, 25.1, 29.3, 32.2 and 33.1.
Assign Miller indices to these lines and decide what type of cubic lattice it is.

(5 marks)

Question Five.

(a) Discuss briefly the free electron approximation in metals. (4 marks)

(b) Assume a plane wave $\psi_k(r) = \exp i(k.r)$, where symbols have the usual meanings, representing a free electron. Use the Schrodinger wave equation to obtain its energy eigenvalues ϵ_k. (4 marks)

(c) (i) What is meant by Fermi energy? (2 marks)

(ii) Use the results in (b) above to show how the Fermi energy is related to the electron concentration, and hence derive an expression for the density of states of the electrons in a metal.

(10 marks)

(d) Calculate the Fermi energy of potassium given that it has a density of $8.6x10^2$ kg m^{-3} and an atomic weight 39. (5 marks)

APPENDIX B
PHYSICAL CONSTANTS

Quantity	Symbol	Value
Angstrom unit	Å	1 Å = 10^{-8} cm = 10^{-10} m
Avogadro number	N	6.023×10^{23}/mol
Boltzmann constant	k	8.620×10^{-5} eV/K = 1.381×10^{-23} J/K
Electronic charge	q	1.602×10^{-19} C
Electron rest mass	m_o	9.109×10^{-31} kg
Electron volt	eV	1 eV = 1.602×10^{-19} J
Gas constant	R	1.987 cal/mole-K
Permeability of free space	μ_o	1.257×10^{-6} H/m
Permittivity of free space	ε_o	8.850×10^{-12} F/m
Planck constant	h	6.626×10^{-34} J-s
Proton rest mass	m_p	1.673×10^{-27} kg
$h/2\pi$	$\hbar$	1.054×10^{-34} J-s
Thermal voltage at 300 K	V_T	0.02586 V
Velocity of light in vacuum	c	2.998×10^{10} cm/s
Wavelength of 1-eV quantum	λ	1.24 μm