

UNIVERSITY OF SWAZILAND.

FACULTY OF SCIENCE.

DEPARTMENT OF PHYSICS.

MAIN EXAMINATION 2006.

TITLE OF PAPER: SOLID STATE PHYSICS.

COURSE NUMBER: P 412.

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 a unit cell of a face centred cubic (fcc) lattice showing the atomic positions of lattice constant 'a'. (2 marks)
- (ii) Find the number of lattice points in the cell. (2 marks)
- (iii) Find the nearest neighbour distance of the lattice. (3 marks)
- (iv) Calculate the packing efficiency of the lattice. (5 marks)
- (b) (i) In the diagram of a cubic unit cell show a (110) and a (100) plane. (4 marks)
- (ii) Calculate the separation between two (123) planes of an orthorhombic cell with $a = 0.82 \text{ nm}$, $b = 0.94 \text{ nm}$ and $c = 0.75 \text{ nm}$ (3 marks)
- (c) A first order reflection from the (111) planes of a cubic crystal was observed at a glancing angle of 11.2° when x-rays of wavelength 154 pm were used. Calculate the length of the side of each cell. (6 marks)

Question Two.

- (a) (i) What is Van der Waals -London attractive interaction in inert gas crystals. (6 marks)
- (ii) Explain how Pauli's exclusion principle is responsible for the repulsive interaction in inert gas crystals. (6 marks)
- (b) (i) Derive the Bragg law $2d\sin\theta = n\lambda$ for diffraction of waves by a crystal lattice. (5 marks)
- (ii) Explain why visible light cannot be used for Bragg reflection. experiments. (2 marks)
- (iii) In the X-ray photograph of a cubic lattice, lines are observed at the following Bragg angles in degrees: 6.6, 9.2, 11.4, 13.1, 14.7, 16.1, 18.6, 19.8. Assign Miller indices to these lines and identify the lattice type. (6 marks)

Question Three.

(a) Given below are that the translation vectors in the direct lattice and the reciprocal lattice respectively: $\mathbf{T} = n_1\mathbf{a} + n_2\mathbf{b} + n_3\mathbf{c}$, $\mathbf{G} = h\mathbf{A} + k\mathbf{B} + l\mathbf{C}$

(i) Write down vectors \mathbf{A} , \mathbf{B} and \mathbf{C} in terms of \mathbf{a} , \mathbf{b} and \mathbf{c} . (2 marks)

(ii) Show that $\exp(i\mathbf{G}\cdot\mathbf{T}) = 1$ (3 marks)

(b) (i) A wave of wave vector \mathbf{k} is incident on a crystal specimen. The diffracted wave has wave vector \mathbf{k}' . Show that diffraction condition for constructive interference between the two waves can be written as: $\mathbf{G} = \Delta\mathbf{k}$, where $\Delta\mathbf{k} = \mathbf{k}' - \mathbf{k}$, where \mathbf{G} is a reciprocal lattice vector.

What is the physical meaning of the above condition?

(9 marks)

$$\text{Given: } n(\bar{r}) = \sum_{\mathbf{G}} n_{\mathbf{G}} \exp i\bar{\mathbf{G}} \cdot \bar{\mathbf{r}}$$

(ii) The geometric structure factor of a crystal is given below :

$$S_{\mathbf{G}} = \sum_{j=1}^s f_j \exp[-i2\pi(n_1h + n_2k + n_3l)], \text{ where 's' is the number of atoms}$$

in the basis and n_1, n_2, n_3 are fractional coordinates. 'f' is the atomic form factor.

Explain the significance of this as regards the identification of lattice type using X-ray diffraction of crystals. Give bcc as an example. (8 marks)

(c) What are Brillouin zones? Draw the first Brillouin zone of a 2-D lattice.

(3 marks)

Question Four.

- (a) (i) Use the Schrodinger wave equation to show how the energy of free electron varies with its wave vector. (6 marks)
- (ii) Sketch a plot of energy E versus the wave vector \mathbf{k} for a free electron. (3 marks)
- (b) (i) According to Kronig-Penny model, energy-wave vector relation for an electron in a periodic potential can be written as:

$$P \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka$$

where ' α ' is a function of energy and 'a' is the width of the potential well.

Take $P = 2\pi$, and for various values of αa , ($\pi/2, \pi, 3\pi/2, 2\pi, 5\pi/2, 3\pi, 7\pi/2, 4\pi$ etc), obtain the LHS of the above expression and sketch a graph against αa .

(10 marks)

- (ii) Sketch a plot of energy versus wave vector \mathbf{k} for an electron in a periodic potential based on observations from the sketch in (b) (i) above and comment.

(6 marks)

Question Five.

- (a) Consider the elastic vibrations of a monatomic crystal. Show that frequency of vibrations of the lattice is given by:

$$\omega^2 = \left(\frac{2c}{M} \right) (1 - \cos Ka)$$

where symbols have their usual meanings. (12 marks)

- (b) (i) Discuss the behaviour of the above relation at the boundary of the first Brillouin zone (3 marks)
- (ii) Simplify the above expression for ω and draw a sketch showing how the frequency ω varies with K in the first Brillouin zone (6 marks)
- (c) Derive an expression for the group velocity of the elastic waves and comment. (4 marks)

PHYSICAL CONSTANTS

Quantity	Symbol	Value
Angstrom unit	\AA	$1 \text{\AA} = 10^{-8} \text{ cm} = 10^{-10} \text{ m}$
Avogadro number	N	$6.023 \times 10^{23}/\text{mol}$
Boltzmann constant	k	$8.620 \times 10^{-5} \text{ eV/K} = 1.381 \times 10^{-23} \text{ J/K}$
Electronic charge	q	$1.602 \times 10^{-19} \text{ C}$
Electron rest mass	m_e	$9.109 \times 10^{-31} \text{ kg}$
Electron volt	eV	$1 \text{ eV} = 1.602 \times 10^{-19} \text{ J}$
Gas constant	R	1.987 cal/mole-K
Permeability of free space	μ_0	$1.257 \times 10^{-6} \text{ H/m}$
Permittivity of free space	ϵ_0	$8.850 \times 10^{-12} \text{ F/m}$
Planck constant	h	$6.626 \times 10^{-34} \text{ J-s}$
Proton rest mass	m_p	$1.673 \times 10^{-27} \text{ kg}$
$h/2\pi$	\hbar	$1.054 \times 10^{-34} \text{ J-s}$
Thermal voltage at 300 K	V_T	0.02586 V
Velocity of light in vacuum	c	$2.998 \times 10^{10} \text{ cm/s}$
Wavelength of 1-eV quantum	λ	$1.24 \text{ }\mu\text{m}$