UNIVERSITY OF SWAZILAND. 107

FACULTY OF SCIENCE AND ENGINEERING

DEPARTMENT OF PHYSICS

SUPPLEMENTARY EXAMINATION 2013/2014

TITLE OF PAPER: SOLID STATE PHYSICS

COURSE NUMBER: P 412

TIME ALLOWED : THREE HOURS

ANSWER ANY FOUR QUESTIONS . ALL QUESTIONS CARRY EQUAL MARKS.

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

Question One 18

(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 $(1\,1\,1), (\bar{1}\,1\,\bar{1}), (1\,\bar{1}\,\bar{1})\,and\,(\bar{1}\,\bar{1}\,1)$. 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)

<u>Question Two</u>

(a) (i) State the main features of ***ionic bonding*** in crystals. Give at least one example. (4 marks)

(ii) What is meant by ***covalent bonding*** in crystals. Give at least one example. (4 marks)

(b) The sodium chloride (NaCl) structure can be regarded as having an fcc lattice with a basis of two ions at 0 and $(a/2)(\hat{x}+\hat{y}+\hat{z})$. Assume that sodium and chlorine ions are hard spheres with radii R_{Na} and $R_{cl.}$

(i) Make a sketch of the ion arrangement in the (100) plane. (2 marks)

(ii) Express the nearest neighbour distance as a function of the lattice parameter 'a.' (2 marks)

(iii) Find the nearest distance between two chlorine ions in terms of 'a'. (2 marks)

(iv) Given that R_{Na} = 0.9 Å and R_{cl} = 1.8 Å, calculate the lattice parameter. (2 marks)

(v) Calculate the fill factor for NaCl. (3 marks)

(c) In an x-ray diffraction experiment using powder method on iron, the first diffraction peak was seen at an angle of 22.3^0. Determine the other possible locations where the diffraction peaks could be seen. (Iron has bcc structure with lattice constant 2.87 Å) (6 marks)

Question Three 195

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

(i) Write down the vectors **A, B** and **C** in terms of **a, b** and **c.** (3 marks)

(ii) Show that exp (i**G.T**) = 1. (2 marks)

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

What is the physical meaning of the above condition?

(10 marks)

[Given: $n(\bar{r}) = \sum_G n_G \exp i\bar{G}.\bar{r}$]

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

$$S_G = \sum_{j=1}^{s} f_i \exp[-i2\pi(n_1 h + n_2 k + n_3 l)]$$, 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. Use a bcc lattice as an example. (10 marks)

Question Four

(a) (i) Use the Schrodinger wave equation to show how the energy of a free electron varies with its wave vector. (6 marks)

(ii) Sketch energy E versus wave vector **k** for a free electron. (3 marks)

(b) (i) According to the Kronig-Penney model, the 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 = 2π, and obtain the LHS of the above expression for various values of αa, ($\pi/2$, π, $3\pi/2$, 2π, $5\pi/2$, 3π, $7\pi/2$,4π etc), and sketch a graph of the LHS against αa.

(10 marks)

(ii) Sketch energy E versus wave vector **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 the frequency of vibrations of the lattice is given by:

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

where the 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)

Appendix 1

Various definite integrals.

$$\int_0^\infty e^{-ax^2}\,dx = \frac{1}{2}\sqrt{\frac{\pi}{a}}$$

$$\int_0^\infty e^{-ax^2}\,x\,dx = \frac{1}{2a}$$

$$\int_0^\infty e^{-ax^2}x^3\,dx = \frac{1}{2a^2}$$

$$\int_0^\infty e^{-ax^2}\,x^2\,dx = \frac{1}{4}\sqrt{\frac{\pi}{a^3}}$$

$$\int_0^\infty e^{-ax^2}\,x^4\,dx = \frac{3}{8a^2}\left(\frac{\pi}{a}\right)^{1/2}$$

$$\int_0^\infty e^{-ax^2}\,x^5\,dx = \frac{1}{a^3}$$

$$\int_0^\infty \frac{x^3\,dx}{e^x - 1} = \frac{\pi^4}{15}$$

$$\int_0^\infty x^{1/2}\,e^{-\lambda x}\,dx = \frac{\pi^{1/2}}{2\lambda^{3/2}}$$

$$\int_0^\infty \frac{x^4 e^x}{(e^x-1)^2}\,dx = \frac{4\pi^4}{15}$$

$$\int_0^\infty \frac{x^{1/2}}{e^x - 1}\,dx = \frac{2.61\pi^{1/2}}{2}$$

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Appendix 2

Physical Constants.

Quantity	*symbol*	*value*
Speed of light	c	3.00×10^{8} ms^{-1}
Plank's constant	h	6.63×10^{-34} J.s
Boltzmann constant	k	1.38×10^{-23} JK^{-1}
Electronic charge	e	1.61×10^{-19} C
Mass of electron	m_e	9.11×10^{-31} kg
Mass of proton	m_p	1.67×10^{-27} kg
Gas constant	R	8.31 J mol^{-1} K^{-1}
Avogadro's number	N_A	6.02×10^{23}
Bohr magneton	μ_B	9.27×10^{-24} JT^{-1}
Permeability of free space	μ_0	$4\pi \times 10^{-7}$ Hm^{-1}
Stefan- Boltzmann constant	σ	5.67×10^{-8} Wm^{-2}K^{-4}
Atmospheric pressure		1.01×10^{5} Nm^{-2}
Mass of $_2^4$He atom		6.65×10^{-27} kg
Mass of $_2^3$He atom		5.11×10^{-27} kg
Volume of an ideal gas at STP		22.4 L mol^{-1}