National University of Singapore

PC3235 Solid State Physics I

(Semester I: AY2010-11, 1 December)

Time Allowed: Two Hours

INSTRUCTIONS TO CANDIDATES

1. This examination paper contains **FOUR** questions and comprises **FOUR** printed pages.
2. Answer any **THREE** questions.
3. Answers to the questions are to be written in the answer books.
4. This is a CLOSED BOOK examination.
5. A Table of Constants is provided.

1. The primitive translation vectors of the hexagonal space lattice are,

$\bar{a}_1 = a\hat{x}$

$\bar{a}_2 = \frac{a}{2}\hat{x} + \frac{\sqrt{3}}{2}a\hat{y}$

$\bar{a}_3 = c\hat{z}$

(i) Calculate the volume of the primitive cell.

[5 marks]

(ii) Derive the primitive translations of the reciprocal lattice $\bar{b}_1$, $\bar{b}_2$, and $\bar{b}_3$ and hence show that the reciprocal lattice vector $G(hkl)$ is:

$$G(hkl) = \frac{2\pi}{a}h\hat{x} + \frac{4\pi}{\sqrt{3}a}\left(k - \frac{h}{2}\right)\hat{y} + \frac{2\pi}{c}l\hat{z}$$

[8 marks]

(iii) Sodium transforms from bcc to hcp at about 23K. Assuming that the density remains fixed through this transition, find the lattice constant a of the hexagonal phase, given that $a = 4.23A$ in the cubic phase and that the c/a ratio is 1.633 in the hexagonal phase.

[6 marks]

(iv) Explain why many metallic elements prefer to be hexagonal closed packed crystal structure.

[6 marks]

2. (a) Consider N atoms at separation a constrained to slide on a circular ring of length L. Use the periodic boundary condition to show that the number of modes per unit range of K is $L/2\pi$ for $-\pi/a \le K \le \pi/a$ and 0 otherwise.

[6 marks]

(b) (i) Derive an expression for the free electron density of states $D(E)$ in (I) 1-dimensional (II) 2-dimensional (III) 3-dimensional metal. Sketch the energy dependence of the $D(E)$ for each case and comment on the results.

[15 marks]

(ii) Sketch a schematic diagram to show density of states with overlapping bands and with a band separated from the others by an energy gap. [4 marks]

3. (a) Starting from the charge neutrality condition, i.e. an uniform semiconductor is electrically neutral, show that the expression for electron concentration is ,

$$N = \frac{1}{2}\left[N_{DD} - N_{AA} + \sqrt{(N_{DD} - N_{AA})^2 + 4n_i^2}\right]$$

where n_i is the intrinsic carrier concentration, N_{DD}, the concentration of donors and N_{AA} the concentration of acceptors. Assume that all the impurities are ionized.

[5 marks]

(b) Assume that valence electrons in the valence band of Ge are following the free electron model. Calculate its valence band width in eV. Note that the conventional unit cell of the diamond structure contains eight atoms. Each atom has 4 valence electrons.

[Lattice Constant of Ge $a = 5.6A$; $\hbar = 1.0546\times10^{-34} Js$; mass of electron $= 9.11\times10^{-31} kg$; $1eV = 1.6022\times10^{-19} J$]

[8 marks]

(c) The Fermi temperature T_F for a particular material $T_F = \frac{E_F}{k_B} = 10000K$ and its Debye temperature is $\theta_D = \frac{\hbar\omega_D}{k_B} = 100K$. The expression for C_v for electron at low temperature is $C_{el} = \frac{1}{2}\pi^2 NK_B \frac{T}{T_F}$ and C_v for phonon at low temperature is $C_{ph} = 234NK_B\left(\frac{T}{\theta_D}\right)^3$.

(i) Derive an approximate qualitative expression for electronic heat capacity for high T.

[3 marks]

(ii) Assuming that classical theory is applicable at high T, obtain an approximate expression for phonon heat capacity at high T.

[3 marks]

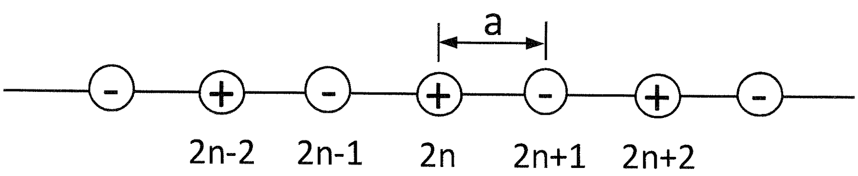
(iii) Estimate the ratio of the two contributions to the specific heat at $T = 1K$ and $T = 400K$. Comment on the results.

[6 marks]

4. Consider a 1-D linear chain composite lattice with two different ions with masses M_+ and M_-. The equilibrium distance between two different ions is a (see figure below). The potential energy between two nearest neighbours is

$$u(r) = -\frac{e^2}{r} + \frac{e^2 b^{n-1}}{n r^n}$$

where e is the charge of the ions; n and b are constants to be determined.



(i) Find the value of b in term of a.

[5 marks]

(ii) Show that the expression of the force constant, β is

$$\beta = (n-1)e^2 a^{-3}$$

[5 marks]

(iii) Write down the equations of motion for displacements of atoms x_{2n+1} and x_{2n+2}.

[5 marks]

(iv) Show that the dispersion relation of the problem is

$$\omega^2 = \frac{\beta}{M_- M_+}\left\{(M_- + M_+) \pm \left[M_-^2 + M_+^2 + 2M_- M_+ \cos(2ka)\right]^{\frac{1}{2}}\right\}$$

[5 marks]

(v) Show that the expression for the sound velocity is

$$v_s = \sqrt{\frac{2(n-1)e^2}{Ma}}$$

where $M = M_+ + M_-$ and you may use $\frac{1}{\mu} = \frac{1}{M_+} + \frac{1}{M_-}$

[5 marks]

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