NATIONAL UNIVERSITY OF SINGAPORE

PC3235 – Solid State Physics I

(Semester I: AY 2018-19)

Time Allowed: 2 Hours

Instructions to candidates

1. Write your student ID on **both** this exam paper (below) **and** the answer books.
2. This exam paper comprises **four (4)** printed pages (including this one).
3. Answer **all ten (10)** questions for **Part I directly on the exam paper**.
4. Answer **all three (3)** problems in **Part II only in the answer book**. Please start each problem in a new page.
5. **At the end, you must submit both your exam paper and answer book**.
6. This is a **closed book** examination but you are allowed to use an A4-sized sheet (both sides) of self-manuscript notes.
7. You can use a non-programmable scientific calculator, but no other electronic devices.

Student ID

Part I (30%, 3% each)

(circle your answers directly here in the exam paper)

All these questions, are written in the standard notation established in our lectures.

1. All Bravais lattices in 2D can be seen as particular cases of the oblique lattice.

   A True   B False

2. The packing fraction of the hexagonal lattice in 2D is

   A $\pi/4$ B $\pi/\sqrt{2}$ C $\pi\sqrt{3}/6$ D $\pi\sqrt{2}/\sqrt{3}$

3. In a simple tetragonal lattice with parameters $c < a$, what is the number of *closest* neighbours to a given atom?

   A 2   B 4   C 6   D 8

4. How many optical branches exist in the phonon dispersion of a crystal with the diamond lattice structure (figure in page 4)

   A 1   B 2   C 3   D 4

5. In Debye's approximation for lattice vibrations, the maximum wavevector k_D for the acoustic phonons is determined from

   A $\frac{4\pi}{3}k_D^3 = N_c\frac{(2\pi)^3}{V}$ B $\frac{4\pi}{3}k_D^3 = \frac{(2\pi)^3}{V}$ C $\frac{4\pi}{3}k_D^3 = \frac{(2\pi)^3}{N_c}$ D $\frac{4}{3}\pi k_D^3 = \frac{N_c}{V}$

6. The Seebeck effect describes the conversion of

   A $\nabla\mu$ into ∇V B $\nabla\mu$ into ∇T C ∇V into $\nabla\mu$ D ∇T into ∇V

7. Bloch's theorem is based on the single assumption of

   A weak potentials   B translation invariance   C an infinite crystal   D rotational invariance

8. A crystal's Fermi surface is entirely contained in the first Brillouin zone. The number of electrons per unit cell must *necessarily* be

   A greater than 2   B less than 2   C less than 1   D greater than 1

9. From the point of view of the tight-binding approximation to the electronic bandstructure, if a crystal is isotropically compressed from its equilibrium state, we expect bandwidths to

   A increase   B decrease   C not change

10. When one substitutes some original atoms in an intrinsic semiconductor and ends up with shallow energy levels in the gap near to the top of the valence band, these are called

    A inert levels   B donor levels   C acceptor levels   D eigen levels

Part II (70%)

(write your solutions only in the answer book)

Problem 1	**crystal lattices and diffraction**	30 % [4, 8, 4, 8, 6]

In an experiment of elastic X-ray scattering, the angle between incoming ($\boldsymbol{k}$) and scattered ($\boldsymbol{k}'$) wavevectors is traditionally designated 2θ.

a) For a given Bragg peak, state the relation between θ and the magnitude of the reciprocal lattice vector $\boldsymbol{G}$ associated with that peak.

b) Powder specimens of three different monoatomic crystals were analysed by X-ray. One is known to have a FCC lattice, one is BCC, and the third has the same crystal structure as diamond. The approximate values of the angles 2θ corresponding to the first diffraction spots are given for each sample in the table below (in degrees).

sample A	sample B	sample C
28.8	42.8	42.2
41.0	73.2	49.2
50.8	89.0	72.0
59.6	115.0	87.3

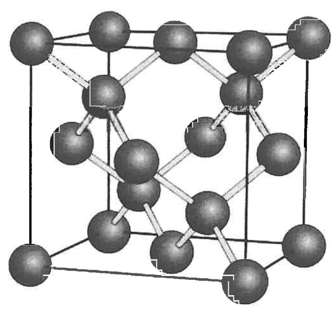
ratio	BCC	FCC
G_2/G_1	$\sqrt{2}$	$2/\sqrt{3}$
G_3/G_1	$\sqrt{3}$	$2\sqrt{2}/\sqrt{3}$
G_4/G_1	2	$\sqrt{11}/\sqrt{3}$

The second table lists the ratio of magnitude of the 4 shortest *reciprocal* vectors to the magnitude of the smallest one ($G_1 = |\boldsymbol{G}_1|$), for crystals with BCC and FCC lattices (such reciprocal vectors have been obtained from the *primitive* vectors of each lattice in real space). Identify the crystal structure of each of the three samples A, B, and C (show your computations).

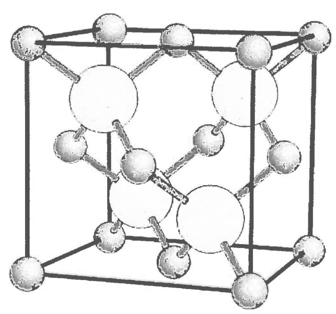
c) Write a set of *primitive* vectors for a FCC lattice whose conventional cubic unit cell has lattice constant a.

d) Show that the ratio G_2/G_1 for the FCC lattice is indeed the value indicated in the table above. *Suggestion: you may expedite the calculation by recalling that the reciprocal vectors of a FCC crystal span a BCC lattice in reciprocal space.*

e) Suppose all the three samples of question (b) had *conventional* unit cells with the same lattice constant a. If a new sample D of zincblende (ZnS) is brought in, also with conventional lattice constant a, at which value of 2θ will we see the first Bragg peak? Justify.



diamond



zincblende

Problem 2	Drude theory	15 % [5, 5, 5]

Drude's classical model, originally developed to describe electronic flow in metals, can be adapted to describe the situation in an insulator. For that, *in addition to* the damping term governed by the relaxation time τ and any external forces, we *add* a restoring force to Drude's equation of motion that is proportional to the deviation of the electron from the origin (like a spring, this force keeps the electron confined to the neighbourhood of its parent nucleus). If an electric field is applied parallel to $\hat{\mathbf{x}}$, that restoring force is

$$F_{\text{res}} = -m\omega_0^2\, x(t),$$

where ω_0 is a characteristic frequency, m the electron's mass, and $x(t)$ is the electron *position*. Consider forces and motion *only* along the direction $\hat{\mathbf{x}}$.

a) Write the equation of motion that describes the time evolution of the electron's *position* in this scenario, in the presence of a generic electric field of magnitude E.

b) Find the solutions of the form $x(t) = x_\omega\, e^{-i\omega t}$ under a time-dependent electric field given by $E(t) = E_\omega\, e^{-i\omega t}$, and determine the relation between the amplitudes x_ω and E_ω.

c) Determine the complex conductivity, $\sigma(\omega)$, which relates the amplitudes of current density and electric field through $J_\omega = \sigma(\omega)\, E_\omega$. What is the value of $\sigma(\omega)$ when $\omega = \omega_0$?

Problem 3	intrinsic semiconductors	25 % [5, 10, 10]

A tight-binding calculation has revealed that the conduction band of an *intrinsic* semiconductor has the following energy dispersion ($t_{x,y,z} > 0$, $a_{x,y,z} > 0$)

$$\varepsilon_c(\boldsymbol{k}) = -2t_x\cos(k_x a_x) - 2t_y\cos(k_y a_y) - 2t_z\cos(k_z a_z).$$

a) Show that, near the bottom of this band, we can approximate

$$\varepsilon_c(\boldsymbol{k}) \simeq E_c + \frac{\hbar^2 k_x^2}{2m_x} + \frac{\hbar^2 k_y^2}{2m_y} + \frac{\hbar^2 k_z^2}{2m_z},$$

and identify what $m_{x,y,z}$ and E_c are in terms of the original parameters $t_{x,y,z}$ and $a_{x,y,z}$.

b) In the approximation of the previous question, derive the density of states (DOS) per spin for this conduction band, $g_c(\varepsilon)$, and *show* it can be written in terms of the DOS of isotropic free electrons, $g^0(\varepsilon)$, if one introduces/defines an effective mass, m_c, for the electrons in this band. Express this effective mass m_c in terms of $m_{x,y,z}$.

c) Unlike the conduction band, this semiconductor's valence band is isotropic near its top:

$$\varepsilon_v(\boldsymbol{k}) \simeq E_v - \frac{\hbar^2 k^2}{2m_v}, \qquad \text{where } E_v < E_c \text{ and } E_c - E_v \gg k_B T.$$

Recalling that the densities of electrons thermally excited to the conduction band, $n(T)$, and holes in the valence band, $p(T)$, are given respectively by

$$n(T) = \frac{2_s}{V}\int_{E_c}^{+\infty} g_c(\varepsilon)\, f(\varepsilon)\, d\varepsilon, \qquad p(T) = \frac{2_s}{V}\int_{-\infty}^{E_v} g_v(\varepsilon)\, \big[1 - f(\varepsilon)\big]\, d\varepsilon,$$

derive the position of the chemical potential as a function of temperature, $\mu(T)$. *Notes: use the quadratic approximation above for both bands; assume that* $\mu - E_v \gg k_B T$ *and* $E_c - \mu \gg k_B T$*; recall that* $n(T) = p(T)$ *in an intrinsic semiconductor. You can leave your result in terms of the conduction band's effective mass,* m_c*. Also,* $\int_0^{+\infty} \sqrt{y}\, e^{-y}\, dy = \sqrt{\pi}/2$.

— **end of exam paper** (*VMP*)