NATIONAL UNIVERSITY OF SINGAPORE

PC3235 – Solid State Physics I

(Semester I: AY 2017-18)

Time Allowed: 2 Hours

Instructions to candidates

1. Write your student ID on **both** this exam paper (below) **and** the answer books. **Do not write your name**.
2. This exam paper comprises **six (6)** printed pages (including this one).
3. Answer **all** the **sixteen (16)** questions for **Part I directly on the test paper**.
4. Answer **all** the **three (3)** problems in **Part II only in the answer books**. In this part, either show your calculations or justify adequately. Please start each problem in a new page.
5. **At the end, you should submit both your exam paper and answer book**.
6. This is a **closed book** examination with authorized materials. Students 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

Physical constants and units (SI)

m_e	$9.109 \times 10^{-31}\,\mathrm{kg}$	k_B	$1.381 \times 10^{-23}\,\mathrm{kg \cdot m^2 \cdot s^{-2} \cdot K^{-1}}$
e	$1.602 \times 10^{-19}\,\mathrm{A \cdot s}$	$\hbar$	$1.054 \times 10^{-34}\,\mathrm{kg \cdot m^2 \cdot s^{-1}}$
N_A	$6.022 \times 10^{23}\,\mathrm{mol^{-1}}$	c	$2.998 \times 10^{8}\,\mathrm{m \cdot s^{-1}}$

$$1\,\mathrm{eV} \simeq 1.602 \times 10^{-19}\,\mathrm{Joule} \simeq 1.160 \times 10^{4}\,\mathrm{Kelvin}$$

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Part I (40 %, 2.5 % each)

(circle or write your answers directly here in the exam paper)

1. How many lattice points (or atoms) are contained in the FCC *conventional* unit cell?

   A one   B two   C three   D four

2. If the inter-ionic distance in a NaCl crystal is 0.28 nm, the *primitive lattice parameter* is

   A 0.14 nm   B 0.56 nm   C 0.07 nm   D 0.40 nm

3. What are the relations among the lattice constants a, b, c, as well as among the angles α, β, γ between the primitive directions in a *tetragonal* Bravais lattice?

   A $\begin{cases} a{=}b{=}c \\ \alpha{=}\beta{=}\gamma{=}90 \end{cases}$ B $\begin{cases} a{=}b{\neq}c \\ \alpha{=}\beta{=}\gamma{=}90 \end{cases}$ C $\begin{cases} a{\neq}b{\neq}c \\ \alpha{=}\beta{=}\gamma{=}90 \end{cases}$ D $\begin{cases} a{\neq}b{\neq}c \\ \alpha{\neq}\beta{=}\gamma{=}\ 90 \end{cases}$

4. If the volume of the primitive cell in a three-dimensional crystal structure is V_c, the volume of its primitive reciprocal cell is

   A $2\pi/V_c$ B $(2\pi)^3 V_c$ C $2\pi V_c$ D $(2\pi)^3/V_c$

5. If q, μ and n represent the charge, mobility and concentration of carriers in a metal, its Drude conductivity is

   A $\sigma = n/\mu q$ B $\sigma = \mu q/n$ C $\sigma = nq/\mu$ D $\sigma = \mu q n$

6. In a Hall effect measurement where a transverse (Hall) field E_y develops under a longitudinal current density J_x and constant magnetic field B_z, the Hall constant is given by

   A $\frac{E_y}{J_x B_z}$ B $\frac{J_x}{E_y B_z}$ C $\frac{B_z E_y}{J_x}$ D $\frac{B_z J_x}{E_y}$

7. Near room temperatures, the Drude relaxation time in a metal depends on temperature as

   A $\tau \propto T$ B $\tau \propto 1/T$ C $\tau = \text{constant}$ D $\tau = 0$

8. At a given temperature, the electron density in silver is $5.86 \times 10^{23}\,\text{cm}^{-3}$ and its resistivity is $1.51\,\mu\Omega \cdot \text{cm}$. What is the Drude relaxation time, in seconds?

   Your response: ________________

9. If the Debye temperature of a crystal is $\Theta_D = 400\,\text{K}$, what is the corresponding Debye frequency, in rad/s?

   Your response: ________________

10. Very close to $T = 0$, the specific heat of a *metallic crystal* varies with temperature as

A $\propto T^3$ B $\propto T$ C $\propto e^{T/\Theta_D}$ D $\propto e^{-T/\Theta_D}$

11. If $\boldsymbol{G}$ represents any reciprocal lattice vector of a crystal whose periodic potential is weak, one expects the appearance of gaps in the electronic energy dispersion *every time* the electron's wavevector $\boldsymbol{k}$ satisfies

A $|\boldsymbol{k}| \ll |\boldsymbol{G}|$ B $\boldsymbol{k} \cdot \boldsymbol{G} = 0$ C $|\boldsymbol{k}| = |\boldsymbol{k} \pm \boldsymbol{G}|$ D $\boldsymbol{k}$ is parallel to $\boldsymbol{G}$

12. The velocity of a Bloch electron belonging to the energy band $\varepsilon_n(\boldsymbol{k})$ is defined as

A $\hbar^{-1}\boldsymbol{\nabla}_{\boldsymbol{k}}\, \varepsilon_n(\boldsymbol{k})$ B $\hbar\boldsymbol{k}/m$ C $\sqrt{2\,\varepsilon_n(\boldsymbol{k})/m}$ D $\hbar\, d\boldsymbol{k}/dt$

13. In order for a crystalline solid to be an insulator, it is *necessary* that the number of electrons per unit cell be

A zero B an odd number C an even number D less than 2

14. The density of electrons in the conduction band of an *intrinsic* semiconductor with band gap E_g varies with temperature as

A $\propto e^{E_g/2k_BT}$ B $\propto e^{-E_g/2k_BT}$ C $\propto E_g/k_BT$ D $\propto (E_g/k_BT)^2$

15. In the context of a tight-binding description of the electronic band structure, if the lattice constant is increased, one expects the width of the electronic energy bands to

A decrease B remain the same C increase

16. In comparison with a partially filled band, the current carried by electrons in a completely filled band is

A the same B larger C zero

Part II (60 %)

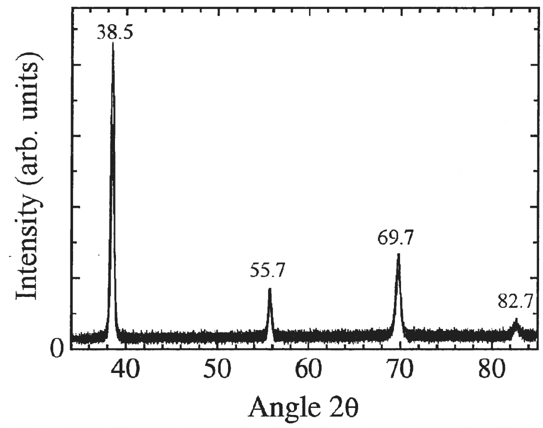
(write your solutions only in the answer book)

Problem 1   20 % [3, 8, 5, 4]

An X-ray diffraction experiment using monochromatic light of wavelength $\lambda = 0.154\,\text{nm}$ was performed on the powder of a crystal whose exterior aspect reveals a *cubic* symmetry. The scattered intensity spectrum obtained as a function of *scattering angle* is plotted in the figure beside, and shows the lowest Bragg peaks recorded at

$$2\theta = \{38.5°,\ 55.7°,\ 69.7°,\ 82.7°\}.$$

This substance is known to be monoatomic.



a) State (or calculate) the lattice structure factors of the body-centred (BCC) and face-centred (FCC) lattices when these are described in terms of conventional cubic unit cells.

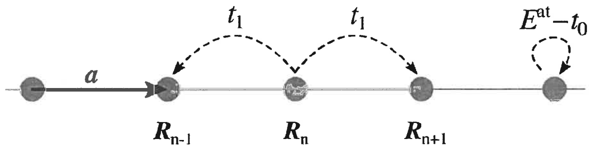
b) Determine whether this crystal has a BCC or a FCC lattice (show your work).

c) Determine the lattice parameter, a, of its *conventional* cubic cell.

d) Determine the volume of the 1st Brillouin zone associated with the crystal's Bravais lattice as a function of the parameter a. [*hint: the crystal is not simple cubic, but you can obtain the result directly from the conventional cubic unit cell*]

Problem 2   15 % [6, 5, 4]

Consider the tight-binding description of a perfect one-dimensional, monoatomic crystal. It is known that only one band crosses the Fermi energy, ε_F, and that band arises from contributions of a *single* atomic orbital at each unit cell, $\phi(r)$.



a) Defining the matrix elements of the Hamiltonian of an electron in the periodic potential as (the hopping amplitudes illustrated in the figure)

$$E^{\text{at}} - t_0 \equiv \langle \phi(0)|\hat{H}|\phi(0)\rangle, \qquad -t_1 \equiv \langle \phi(a)|\hat{H}|\phi(\pm a)\rangle, \qquad (t_1 > 0)$$

obtain the analytical expression for the electronic band dispersion, $\varepsilon(k)$, in the nearest-neighbour, orthogonal tight-binding approximation.

b) Determine ε_F when the number of electrons in this band amounts to 1 per unit cell.

c) For such value of ε_F, is this an electrical conductor or an insulator? Justify.

Problem 3	25 % [3, 4, 6, 8, 4]

Consider the description of *free* electrons in a piece of metal with volume V according to Sommerfeld's theory (in 3 dimensions).

a) Derive the density of electronic states per spin (DOS), $g(\varepsilon)$, for free electrons.

b) State how the volume density of electrons, n_e, is related to the DOS. Hence, or otherwise, obtain the Fermi energy, ε_F, as a function of n_e.

c) If the electronic density is kept constant, derive how the chemical potential, μ, deviates from ε_F as a function of temperature, to lowest order in temperature. Express your result in terms of the DOS. [*hint: use Sommerfeld's expansion; also, it's better to keep $g(\varepsilon)$ unspecified throughout your steps and final result*]

d) The thermal conductivity, κ, relates the heat flux that results from a temperature gradient through $\boldsymbol{J}^q = -\kappa \, \boldsymbol{\nabla} T$. It can be calculated within Drude-Sommerfeld theory from

$$\kappa = \frac{2\tau}{3Vm} \frac{\partial}{\partial T} \sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}}^2 \, f(\varepsilon_{\boldsymbol{k}}),$$

where τ is the relaxation time (assumed to be $\boldsymbol{k}$-independent), $\varepsilon_{\boldsymbol{k}}$ the free electron energy dispersion, m the electron's mass, and $f(\varepsilon)$ represents the Fermi-Dirac distribution. Show that, to lowest order in a Sommerfeld expansion, the above expression leads to

$$\kappa \simeq \frac{\pi^2 n_e \tau k_B^2 T}{3m}.$$

[*hint: you will need the result of question c; also, do $\partial/\partial T$ only at the end*]

e) Compute κ at $T = 300\,\mathrm{K}$ for a metal whose Drude resistivity is $1.7\,\mu\Omega \cdot \mathrm{cm}$ at that temperature. Present the magnitude of your final result in SI units.

Note: recall that the lowest orders of the Sommerfeld expansion are

$$\int_{-\infty}^{+\infty} H(\varepsilon) f(\varepsilon)\, d\varepsilon = \int_{-\infty}^{\mu} H(\varepsilon)\, d\varepsilon + \frac{\pi^2}{6}(k_B T)^2 H'(\mu) + \frac{7\pi^4}{360}(k_B T)^4 H'''(\mu) + \mathcal{O}(T^6).$$

— **end of exam paper** (*VMP*)