Introduction to Solid State Physics - NTU/Grad. Inst. Appl. Phys. – 博士資格考試 – March 2015

[**Total points 100**]

1. [**6 pts**] What are Bragg and Von Laue formulations of x-ray diffraction by a crystal? Demonstrate the equivalence of the Bragg and Von Laue formulations.

2. [**Crystal Structure and Reciprocal Lattice, 24 points**]

(a) What is a primitive cell? **[1pts]**

(b) What is the Wigner-Seitz primitive cell? **[1pts]**

(c) Write down the five Bravais lattices in two dimensions. You may describe them using drawings with axes and angles. **[3 pts]** Show that their Wigner-Seitz cell is either a hexagon or a rectangle. **[1pts]**

(d) Figure 1 is an FCC (face-centered cubic) lattice. Given by a set of basis vectors, the indices of crystal planes can be determined. For example, (100), (110) and (111) crystal planes are determined with the bases of $\vec{a} = a\hat{x}$, $\vec{b} = a\hat{y}$, $\vec{c} = a\hat{z}$. What are the new indices if $\vec{a'}$, $\vec{b'}$, $\vec{c'}$, as described in Fig. 1, used as the new bases? Please write the crystal planes, respectively. **[3 pts]**

(e) we now choose $\vec{a'}$, $\vec{b'}$, $\vec{c'}$ as our bases but re-name them as $\vec{a_1}$, $\vec{a_2}$, $\vec{a_3}$ respectively, Write down $\vec{a_1}$, $\vec{a_2}$, $\vec{a_3}$ in vector form (i.e. using $\hat{x}$, $\hat{y}$, $\hat{z}$). **[1pts]**

(f) Construct the corresponding reciprocal bases $\vec{b_1}$, $\vec{b_2}$, $\vec{b_3}$ (need calculation). **[2 pts]**

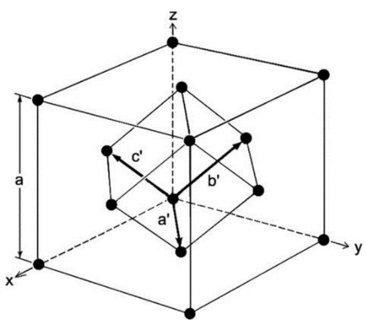
(g) What is the packing fraction of fcc lattice? **[2pts]**

(h) What is the lattice structure of fcc lattice in the reciprocal space? **[2pts]**

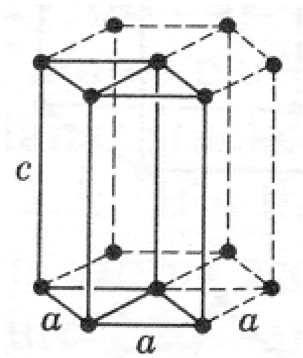
(i) Figure 2 on the right-hand side is an hcp (hexagonal closed-packed) lattice. Choose a proper primitive vectors to show that its reciprocal lattice is also a simple hexagonal, with lattice constant $2\pi/c$ and $4\pi/\sqrt{3}a$, rotated through 30^o about the c-axis with respect to the direct lattice. **[2pts]**

(j) For what value of c/a does the ratio have the same value in both direct and reciprocal lattices? **[2pts]** What is the ideal c/a ratio **[2pts]** If c/a is ideal, what is its value in the reciprocal lattice? **[2pts]**

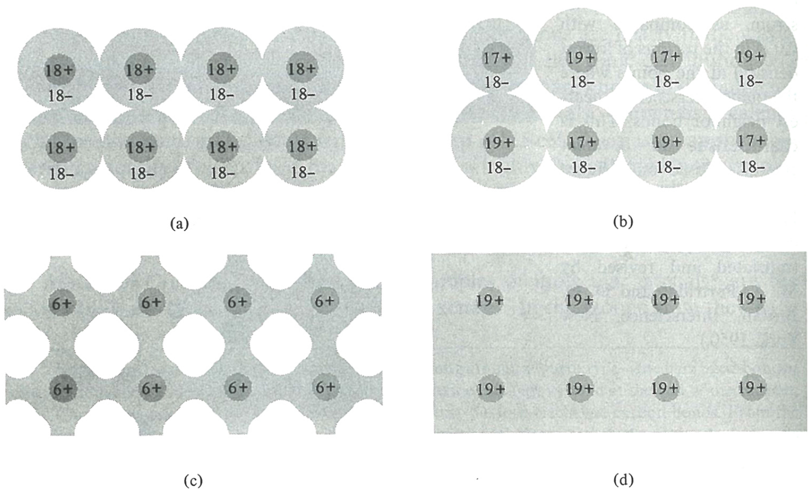
(Fig.1)



(Fig.2)



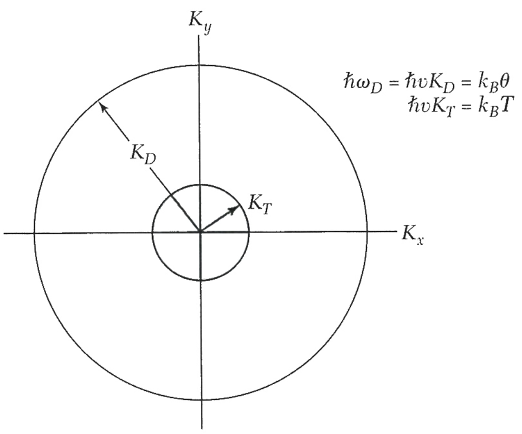
3. [**15 pts**] (a),(b),(c),(d) is the illustration of four different types of crystal binding with positive cores and surrounding negative electrons. The charge of the positive cores and negative electrons are stated by numbers. Please identify the types of crystal binding for each image (**2 pts**) and give thorough explanation on the four binding forms (**7 pts**). Furthermore, please give a material system from each crystal binding. (**2 pts**) (c) From the Lennard-Jones potential, we know that in this model the cohesive energy should be all the same for Ne, Ar, Kr, Xe. Please explain why the observed boiling points (melting points) of these four inert gases are different (**2 pts**). Crystal structures have been studied through diffraction of photons, neutrons, and electrons. Please describe the studies as much as you know and the differences among the three types of diffraction. (**2 pts**)



4. [**15 pts**] At temperature much below the Debye temperature and the Fermi temperature, the heat capacity can be written as the sum of the electronic and phonon contributions as

$$C/T = \gamma + AT^2$$

   (a) Explain the failure of the classical Drude Model and the success of the Sommerfeld theory to give the correct expression for the electronic heat capacity. (**5 points**)
   (b) Derive the T-linear dependence of the electronic heat capacity term using a qualitative approach based on the Fermi Dirac distribution function for the free electron gas. (**5 points**)
   (c) Derive the ***Debye T^3 –law*** for the phonon heat capacity term by using a qualitative approach for the allowed excited phonon modes in the ***K*** – space. (**5 points**)



5. [**20 pts**] In the free electron gas model, the electron transport follows the so called the Ohm's law.

(a) Derive the Ohm's law to express the electrical conductivity as

J = σ E, where **σ = ne²τ/m,** and τ is the collision time. **[4 points]**

(b) The mobility is defined as the ratio of the drift velocity to the electrical field as μ = υ/E. Show that the electrical conductivity to be related to μ as **σ = neμ**, and **μ = eτ/m** **[4 points]**

(c) The thermal conductivity ***K*** of a solid is defined with respect to the steady law of heat down a long rod with a temperature gradient ***dT/dx***, where j_U is equal to $-K\, dT/dx$, and j_U is the thermal energy transmitted across per unit area per unit time. Show that thermal conductivity is given as ***K = 1/3 C v l,*** where ***C*** is the heat capacity per unit volume, *υ* is the average particle velocity, and ***l*** is the mean free path between collisions. **[4 points]**

(d) Following the equation for total heat capacity in the problem ***4***, the explicit expression for γ is $\frac{1}{2}\pi^2 N k_B Z/T_F$, where T_F is the Fermi temperature. Derive the electron thermal conductivity to be $K_{el} = (\pi^2 n\, k_B^2 T\tau)/3m$ **[4 points]**

(e) Taking the ratio of electron thermal conductivity to electrical conductivity, and derive the **Wiedemann – Franz Law and the Lorentz number**. **[4 points]**

6. [**20 pts**] Bloch theorem states that the solutions of Schrodinger equation for a periodic potential can be written down in a special form called Bloch functions.

(a) What is the form of a Bloch function. **[2 points]**

(b) Give an argument that Bloch functions are indeed solutions of Schrodinger equation for a periodic potential. This is the same as the proof of Bloch's theorem. **[10 points]**

(c) What is the origin of the energy gap in the solids. **[2 points]**

(d) The energy gaps for semiconductors are all temperature-dependent. Give main sources of this temperature dependence. **[2 points]**

(e) The following equation is the solution of delta-function potential Kronig-Penny model (periodicity of a). If now P is far less than 1, find the lowest energy at $\mathrm{k} = 0$. **[2 points]** For the same problem, find the first band gap at $\mathrm{k} = \pi/a$. **[2 points]**

$$\frac{P}{Ka}\sin Ka + \cos Ka = \cos ka, \text{ with } \epsilon = \frac{\hbar^2 K^2}{2m}, \text{ k in the first zone and P constant}$$