Introduction to Solid State Physics - NTU/Grad. Inst. Appl. Phys. – 博士資格考試 – Feb. 2016

[Total points 120]

[1. Crystal lattices, reciprocal lattices, and diffraction, 25 points]

A fundamental concept in the description of any crystalline solid is that of Bravais lattice, which specifies the periodic array in which the repeated units of the crystal are arranged.

(*3pts*)(a) How many distinctive lattice types in three dimensions and what are they?

(*2pts*)(b) What is a primitive cell? What is a Wigner-Seitz cell?

(*2pts*)(c) What is the reciprocal lattice to a bcc lattice? Show the calculation.

(*6pts*)(e) Calculate the structure factors in the x-ray diffraction from (i) bcc, (ii) fcc, and (iii) diamond.

(*3pts*)(f) Prove that in a cubic crystal a direction [*hkl*] is perpendicular to a plane (*hkl*) having the same Miller indices. What is the distance between each successive plane?

(*3pts*)(g) 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.

(*6pts*) 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. Free electron Fermi gas, 15 points]

(*2pts*)(a) Draw Fermi distributions $f(\varepsilon) = \frac{1}{e^{(\varepsilon-\mu)/k_BT}+1}$ as functions of ε with temperature at room temperature $(k_BT \sim 0.01\mu)$ and very high temperature of $k_BT \sim 0.5\mu$.

Sommerfeld modified the Drude model and hence got a better improvement of metal properties:

(*1pt*)(b) What is the modification made by Sommerfeld on the Drude model?

(*3pts*)(c) Show that the kinetic energy of a three-dimensional gas of N free electrons at T = 0K is $U_0 = \frac{3}{5}N\varepsilon_F$.

(*2pts*) (d) Now consider a 2-dimensional electron gas system, what is the relation between n and k_F

(*2pts*) (e) Derive the density of levels g(ε) in 2-dimentional electron gas.

(*5pts*) (f) Derive the relationship between μ and ε_F in 2-dimensional case.

[3. Crystal binding, 15 points]

(*5pts*)(a) What are the principal types of crystalline binding? Give at least two material systems to each type.

(*10pts*)(b) Lennard-Jones potential is a simple model to estimate the total energy of an inert gas crystal and has the form $U_{tot} = 2N\varepsilon[\sum_j' \left(\frac{\sigma}{p_{ij}R}\right)^{12} - \sum_j' \left(\frac{\sigma}{p_{ij}R}\right)^6]$. (i) Please give an explanation to the meaning (what causes each of these terms...) of the first and second terms in the Lennard-Jones potential. (**2pts**) (ii) For fcc structure, we know $\sum_j' p_{ij}^{-12} \approx 12.132, \sum_j' p_{ij}^{-6} \approx 14.454$. Calculate the equilibrium nearest-neighbor distance (**3 pts**) and the cohesive energy (**3 pts**) for inert gas crystal in fcc structure (Ne, Ar, Kr, Xe). You will discover that in this simple model the equilibrium nearest-neighbor distance and cohesive energy is the same for these four inert gases. (iii) From (ii), we know that in this model the cohesive energy should be all the same. Please explain why the observed boiling points (melting points) of these four inert gases are different (**2 pts**).

	Neon	Argon	Krypton	Xenon
Boiling point (K)	27.3	87.4	121.5	166.6
Melting point (K)	24.7	83.6	115.8	161.7

[4. Bloch electrons and energy band theory, 25 points]

(a) What is Bloch's Theorem? **[2 points]** (b) Prove it. (You may prove it from general quantum-mechanical consideration or other considerations.) **[5 points]** *[Hint: You may try to construct a displacement operator of the wave function, and consider the commutation relation with Hamiltonian]*

(b) In the free electron model, we cannot explain why there are insulator and semiconductor because we do not have the concept of energy gap at that time. Please compare the difference between free electron model and nearly free electron (Bloch electron) model, and explain the origin of the energy gap. (You do not need to give out a throughout calculation to prove the existence of energy.) **[3 points]**

(c) In Bloch electrons, $\hbar\kappa$ is known as the crystal momentum of the electron, to emphasize its similarity, but one should not be misled by the name $\hbar\kappa$ into thinking that is a momentum, for it is not. Explain it. **[3 points]**

(d) The wave vector κ appearing in Bloch theorem can always be confined to the first Brillouin zone. Explain it. **[3 points]**

(e) Kronig-Penney Model. (a) For the delta-function potential and with P being far less than 1 (<<1), find at k =0 the energy of the lowest energy band. **[4 points]** (b) For the same problem find the band gap at k=π/a. **[5 points]**
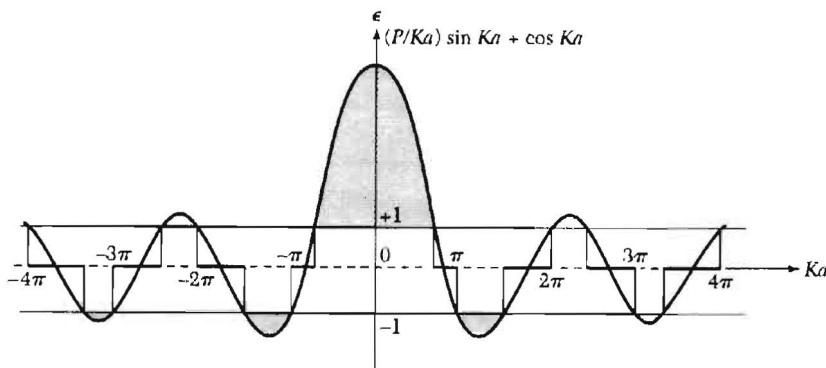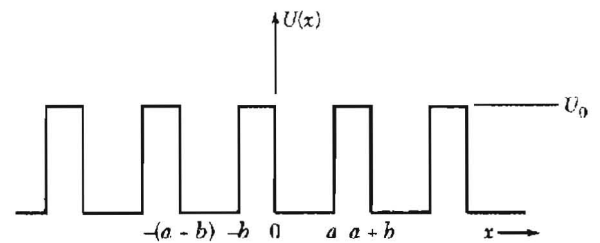

Figure 5 Plot of the function $(P/Ka) \sin Ka + \cos Ka$, for $P = 3\pi/2$. The allowed values of the energy e are given by those ranges of $Ka = (2me/\hbar^2)^{1/2}a$ for which the function lies between ±1. For other values of the energy there are no traveling wave or Bloch-like solutions to the wave equation, so that forbidden gaps in the energy spectrum are formed.

Square-well periodic potential as introduced by Kronig and Penney.

[5. Semiconductor crystals, 25 points]

(a) Why the electrical conductivity of a semiconductor increases with increasing temperature while that of a metal decreases? **[2 points]**

(b) Give at least two semiconductors with one having direct-gap and another having indirect-gap. Explain the direct absorption process and indirect absorption in the two semiconductors. **[3 points]**

Explain the temperature dependence of the energy gaps in semiconductors. **[3 points]**

(c) Explain holes in semiconductors. How do they behave electrically? **[3 points]**

(d) Derive the effective mass equation $(\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2\varepsilon}{dk^2})$ from the equations of motion for Bloch electrons in the Semi-classical model of electron dynamics. **[3 points]**

$$v_g = \hbar^{-1}\frac{d\varepsilon}{dk}, \quad \hbar\frac{d\vec{k}}{dt} = \vec{F}$$

(e) What is the mobility of a semiconductor for electrons and holes and how is it measured? **[3 points]** In a perfect semiconductor with no defects and no impurities, what is the mobility at low temperatures where lattice vibration (phonon effect) is extremely small. **[3 points]**

(f) What are the donors and acceptors in semiconductors? **[2 points]** (You may use Si as an example) Explain the donor energy levels which are close to the bottom of the conduction band. **[3 points]**

[6. Phonons, 15 points]

The Debye model assumes that heat capacity of a solid comes from the excitation of acoustic phonons. Consider a solid of volume V containing N primitive cells, with only one atom in each primitive cell, and the dispersion relation is given $\omega = vk$ for each polarization.

(a) Find the expression for Debye frequency ω_D in one polarization. **[4 pts]**

(b) Derive the heat capacity of the solid at high temperature regime such that Dulong-Petit law can be explained. **[6 pts]**

(c) Briefly describe the Einstein model. **[2 pts]**

(d) Compare the lattice and electronic specific heats. **[3 pts]**