Final Exam - Solid State Physics 1

Wednesday, 22nd of January 2020, 8:30-11:30 AM

This is a closed book exam. You are not allowed to bring books, notes *etc*. You can use a basic or scientific calculator, but no other electronic equipment having capabilities to display the course content.

Each sub-question is independently solvable. Work on the easy questions first and earn the bonus points as your final step!

Do not forget to write your **full name** and **student number** on **each** sheet that contains your answer. Please write in a clear way!

The exam has 4 questions with a total of 100 points plus 10 bonus points.

This has exam has been drafted by J. Ye and verified by G. Blake

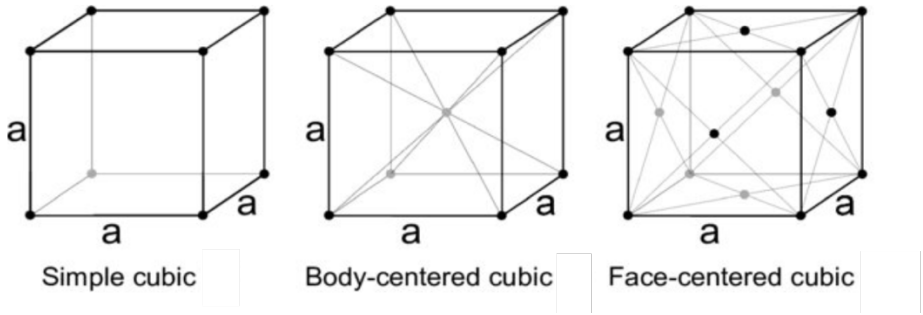
Date: 18/01/2020 Date: 18/01/2019

J. Ye G. Blake

----------**The Start of Questions**----------

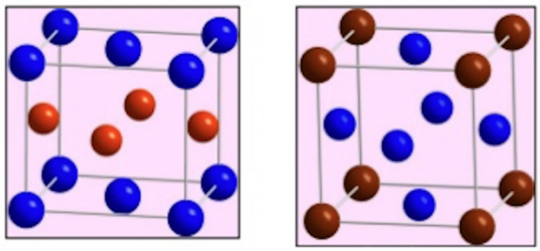
Question 1: Crystal structure (25+3 points)

A. Cubic Lattice systems has three structures shown below

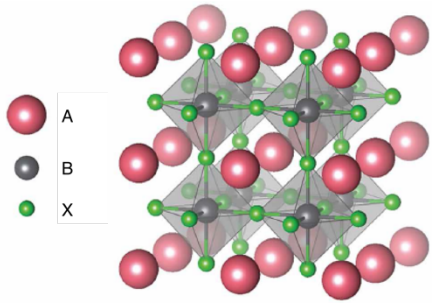


1) (**9p**) Two-dimensional (2D) Bravais lattices can be generated by cutting lattice planes of a 3D Bravais lattice. Determine the 2D Bravais lattices for the (100) (110) and (111) planes of simple cubic, body-centered cubic, and face-centered cubic crystals. Determine the lengths of ***i***, ***j*** in the unit of a, and the angle θ between ***i*** and ***j***.

2) **(6p)** Changing the stoichiometry of intermetallic alloy, A_xB_y, can form different crystal phases. For example, change the ratio of Au (blue ball)/Cu (brown ball) can form the two crystal structures shown below. Identify which one is the AB and which one is the AB_3 phase, Determine the Bravais lattice and number of basis atoms for these two crystals (hint: the atoms in the primitive cell should reflect the stoichiometry).



A perovskite: ABX_3 has a general crystal structure as shown below, where A, B, and X are labeled for different atoms or molecules.

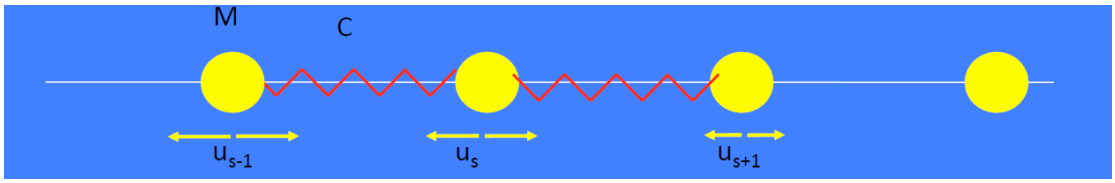


3) (**4p**) Use the idea of repeating environment (say you choose the environment of atom A as the environment to be repeated), identify the Bravais lattice and number and kind of atoms (as A, B, or X) in the basis.

4) (**2p**) Calculate the volume of the primitive cell in terms of a between neighboring X atoms.
5) (**4p**) Setup a coordinate system, and calculate the phase factor after summing up $f_i e^{i\phi_i}$ from the i^{th} atom in the basis and determine the scattering intensity by using f_A, f_B, and f_X.
6) (**3p bonus**) Some ABX_3 compounds are composed of atoms with very different scattering atomic form factors. For example, $CH_3NH_3PbI_3$ is a highly efficient candidate for solar cells, where the $(CH_3NH_3)^-$ ion replaces the A atom in the ABX_3 structure. If the scattering from light atoms can be ignored, re-analyze the problem above for this solar cell material. (electronic configurations are H: $1s^1$, C: $2s^2 2p^2$, N: $2s^2 2p^3$, Pb: $6s^2 6p^2$, I: $5s^2 5p^5$)

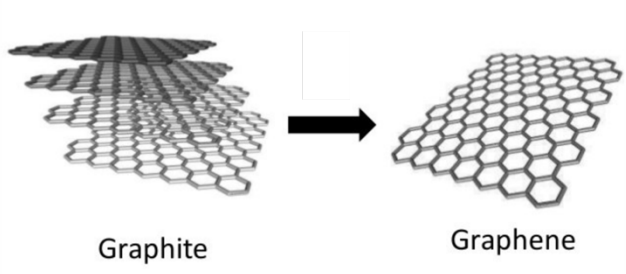
Question 2: Phonons and thermal properties (25+3 points).

As shown below, consider a linear chain of N atoms all with mass M, and force constant C.



1) (**6p**) Calculated and sketch the dispersion relation in the first Brillouin zone for the chain above.

2) (**6p**) From the dispersion relation, show that the density of modes $D(\omega) = \frac{2N}{\pi}\frac{1}{\sqrt{\omega_m^2-\omega^2}}$, where ω_m is the maxim frequency ($\sin^2 x + \cos^2 x = 1$).
3) (**6p**) Suppose the optical branch has the form of $\omega(K) = \omega_0 - AK^2$ near $K = 0$, where ω_0 is a constant. In three-dimension case, show that $D(\omega) = (\frac{L}{2\pi})^3 \frac{2\pi}{A^{\frac{3}{2}}}\sqrt{\omega_0 - \omega}$ for $\omega < \omega_0$, and $D(\omega) = 0$, for all $\omega > \omega_0$.
4) (**3p**) Sketch the dispersion relation in the first Brillouin zone if either the force constant or the mass of atoms changes so that the mono-atomic chain becomes a di-atomic chain. How will the $\omega(k)$ relationship evolve?
5) (**4p**) If the number of atoms in the basis increases from 2 to $n = 3, 4, \ldots$, describe the change to the BZ and how many vibration modes and optical modes can you have if we consider both longitudinal and transverse modes?
6) (**3p bonus**) Consider a simplified model of graphite, which is composed of graphene layers as shown below. The motion of the atoms is restricted to the plane of the carbon layer. Show that the phonon heat capacity in the Debye approximation in the low-temperature limit is proportional to T^2.

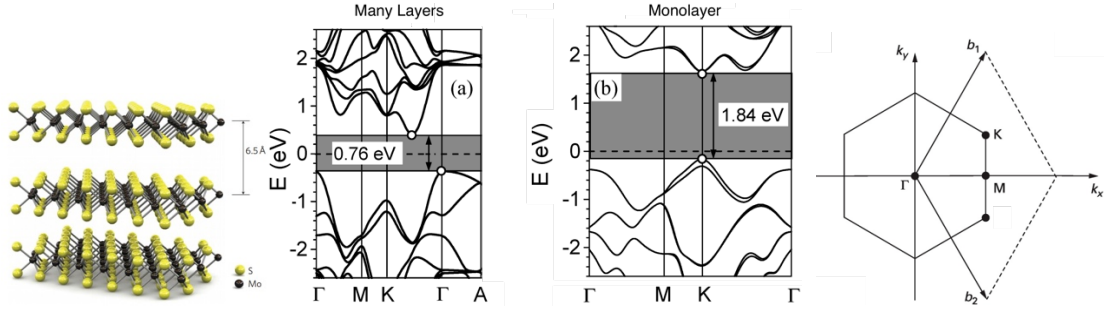


Question 3: Free electrons in Copper and its alloys (25+2 points)

Copper is a typical metal with $3d^{10}4s^1$ configuration. The Fermi energy of electrons in FCC copper single crystal is 7.0 eV at room temperature. From Hall effect measurements, the electron drift mobility in copper is 33 $cm^2V^{-1}s^{-1}$.

1) (**5p**) What is the speed v_F of conduction electrons with energies around E_F in copper? By how many times is this larger than the average thermal speed v_{th} of electrons, if free electrons behave like an ideal gas? (Maxwell-Boltzmann statistics and $E = 3k_BT/2$)
2) (**2p**) Why is v_F much larger than v_{th}?
3) (**3p**) What is the De Broglie wavelength of these electrons? ($p = \hbar k$ and $\lambda = 2\pi/k$)
4) (**4p**) Will the electrons get diffracted by the lattice planes in copper, given that interplanar separation in Cu = 2.09 Å (try the Bragg's law here for electrons)?
5) (**3p**) Discuss the main similarities and differences between Drude's and Sommerfeld's models for the free electrons. What was added in the latter model for the calculation of specific heat of free electron?
6) (**4p**) In the electromagnetic field, the force on a charged particle is $F = q(\boldsymbol{E}+\boldsymbol{V}\times\boldsymbol{B})$. Calculate and sketch the change of momentum of the electrons due to the electric field $\boldsymbol{E}$ for the 3D free electrons in a metal.
7) **(2p bonus)** What will happen to the Fermi sphere above if both $\boldsymbol{E}$ and $\boldsymbol{B}$ fields are applied.
8) (**4p**) If FCC lattice constant $\boldsymbol{a}$ = 3.597 Å, suppose you can make a 2D metal film by cutting a lattice plane of a copper single crystal for the (001) plane, calculate and draw the Fermi surface of your mono-atomic thick Cu film.

Question 4: Semiconductor, magnetism, and superconductivity (25+2 points)



Like graphene in question 2(6), a 2D semiconductor can be isolated from a material called MoS_2 (shown above). The band structure of the system evolves with the number of layers. As shown above, the monolayer MoS_2 is a 2D system with a hexagonal first Brillouin zone (BZ).

1) **(6p)** From the band structures above for the many-layer and monolayer MoS_2, find the

location (at which point or between which points of the BZ) of conduction and valence band edge in the first BZ. Identify the size and characteristic of the band gap (direct or indirect) for these two systems.

2) (**5p**) Discuss the energy and momentum conservation in the optical absorption of monolayer and many-layer MoS_2. Sketch the optical absorption of MoS_2 near the band edge as the function of the energy of the incident photons for both many-layer and monolayer cases.

3) (**4p**) From the Newtonian law, $F = ma = -dU/dx$, Express the effective mass from the dispersion relationship $E(k)$.

4) (**6p**) Free electrons can be induced in MoS_2 either by impurity doping or field-effect gating. Sketch the band diagram of having free electron in the conduction band by impurity doping. Sketch the change to the density of states when free electrons a monolayer MoS_2 is subjected to a magnetic field $\boldsymbol{B}$? Mark the spin quantum number S_z and magnetic moment on the density of states (hint: monolayer MoS_2 is a 2D system).

5) **(4p)** Consider MoS_2 as a nonmagnetic matrix, magnetic ions can be doped to induce ordered magnetism in the system. If we choose Cr^{2+} (4 electrons in the *d* shell), and Fe^{2+} (6 electrons in the *d* shell) ions as the dopant to MoS_2. Determine the magnetic configuration $^{2S+1}L_J$ for these ions using Hund's rule.

6) **(2p bonus)** If we dope MoS_2 with a sufficient amount of carriers by field-effect gating, the free electrons eventually turns superconducting. What are the two hallmark physical properties that differentiate a superconductor from any other conductor? If the magnetic lines can pass the monolayer at defects, sketch the magnetization *M*, and internal field *B* of a monolayer MoS_2 as a function of external field $\mu_0 H$ applied perpendicular to the plane of MoS_2.

----------The End of Questions----------