

Electrons in crystals
I test - 4 November 2008
(2 hours)

Exercise: Free electrons

Sodium (Na) in standard temperature and pressure conditions is a metal with BCC structure, density of about 0.97 g cm^{-3} , mass number = 23 and Fermi energy $E_F=3.24 \text{ eV}$.

1. Calculate the Fermi temperature T_F .
2. Calculate the Fermi velocity v_F and the kinetic energy at $T=0^\circ \text{ K}$.
3. Calculate the kinetic energy variation at room temperature (Hint: Sommerfeld expansion)
4. If the electron gas is instead treated as a classical one, which is the kinetic energy at $T=0^\circ \text{ K}$? and at room temperature?
5. Using the given Fermi energy, calculate the free electron density n .
6. Calculate the atomic density (number of atoms per unit volume) of solid sodium and the average free electrons per atom. Is it the result you were expecting?
7. From the electron density calculated in (5.), calculate the plasma frequency.
8. Given the resistivity in DC at room temperature, $\rho= 4.2 \mu\Omega \text{ cm}$, calculate the relaxation time τ and the electron mean free path ℓ .
9. At which frequency the *real* part of the conductivity in AC will be 1/5 of its zero-frequency value?

Exercise: *Crystalline structures*

1. Determine the atomic density in the crystalline planes (001), (110) and (111) in the FCC structure as a function of the lattice parameter (side of the cubic cell) a_0 .
2. Given that Cu has a FCC structure with $a_0=3.61 \text{ \AA}$, calculate explicitly the atomic density in the (110) plane.
3. Calculate the packing fraction of FCC structure.

Exercise: *Miller indices, distances among crystalline structures, diffraction*

1. Calculate the interplanar distance of the families of planes (100), (110), (111) and (211) of a cubic crystal as a function of the lattice parameter a_0 .
2. Consider $a_0 = 2.62 \text{ \AA}$. Determine the Bragg angle corresponding to the reflection from the families of planes (100), (110), (111) and (211), for an incident wavelength $\lambda=1.54 \text{ \AA}$.
3. Knowing that with the same λ , the Bragg reflection angle from the (110) planes in Fe (BCC structure) is 22° , calculate the Fe lattice parameter.

Exercise: *Diffraction from a linear biatomic chain*

Consider a linear chain of atoms ABABA...AB, with bond length A-B equal to $a/2$ and atomic form factors f_A and f_B for A and B atoms respectively. The incident X-ray beam is perpendicular to the linear chain.

1. Show that the condition of constructive interference is $n\lambda = a \cos \theta$, where θ is the angle between the diffracted beam and the atomic chain.
2. Show that the intensity of the diffracted beam (under conditions of constructive interference) is proportional to $|f_A - f_B|^2$ for n odd and $|f_A + f_B|^2$ for n even.
3. Discover and comment what happens for $f_A = f_B$.