Homework - Week 10

Exercise 1 – The Aluminium crystal

In a piece of aluminium, atoms are arranged in a face-centered cubic (fcc) structure with lattice constant $a = 4.05$ angstrom.

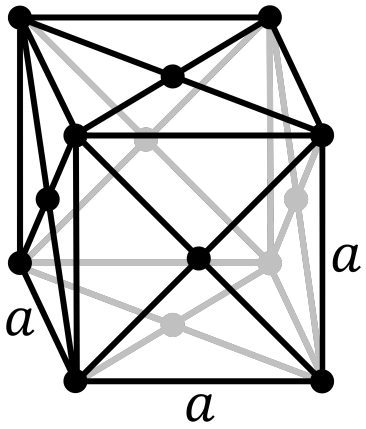

Figure 1: Conventional cell for the fcc lattice.

1. Estimate the density (gr/cm^3) of Aluminium.
   (*Hint*: the atomic weight for Aluminium is about 27u, where the atomic mass unit is $1\text{u} = 1.66 \times 10^{-27}$ kg).
2. Compute the distance between the nearest-neighbour atoms.

The close–packing condition corresponds to distributing solid spheres at each site of a Bravais lattice in such a way that neighboring spheres just touch, without overlapping. In this context, the packing fraction is the fraction of volume in a crystal occupied by the spheres satisfying the close–packing condition.

3. Compute the radius of the spheres that satisfy the close–packing condition for the fcc lattice of Aluminium.
4. Compute the packing factor for the fcc lattice (i.e. the ratio of volumes occupied by the spheres and the volume of the cell).
5. By knowing that the density of free electrons in aluminium is $\rho_{free} = 2.1 \times 10^{29}$ m^{-3}, estimate the oxidation state of bulk aluminium, and compare it with the nominal value (3+).

   Oxidation state describes how many electrons can be lost or gained by an atom in a chemical compound.

   Hint: Compute the ratio between ρ_{free} and the density of atoms: $(N_{atoms/cell})$ / V_{cell}.

Exercise 2 – Electrons in an empty lattice

Consider a free electron gas in a one-dimensional box of size L in periodic boundary conditions (PBC) with an empty (zero potential) lattice of width a with N cells.

1. Write the Hamiltonian and find eigenvalues and eigenvectors.

   (*Hint for the eigenvectors: choose between those plain-waves that are compatible with PBC.*)

2. Do the eigenvectors satisfy Bloch theorem? Check the hypotheses.

   (*Hint: Is the potential periodic?*)

3. To check if the thesis of Bloch theorem is compliant for this particular problem, we must observe that the k labeling the plain-waves found in point (1) is not quite the same as the one of Bloch functions. The k of Bloch functions is defined to be inside the first Brillouin zone (because it is the label of the eigenvalues of the translations). With this in mind, for the eigenfunctions found previously prove the second of the two equivalent statements of the thesis of Bloch theorem, i.e. the relation:

   $$\psi_k(x) = e^{ikx} u_k(x), \tag{1}$$

   where $\psi_k(x)$ is the eigenfunction of the hamiltonian and $u_k(x)$ is a function with the same periodicity of the lattice.

   How does the band structure (*i.e.* the energy dispersion as a function of the Bloch's k) look like for a free electron gas in one dimension?

4. Determine the electrons' mean velocity for the lowest energy band at the center and at the boundary of the first Brillouin zone.

   (*Hint: The electrons' mean velocity is defined as* $\frac{1}{\hbar}\frac{\partial \epsilon}{\partial k}$*, where* ϵ *is the band energy.*)

Exercise 3

The electronic band structure and the density of states (DOS) are important properties which allow us to understand basic aspects of the behavior of materials. In the following, we will consider band structure plots and DOSs from actual calculations.

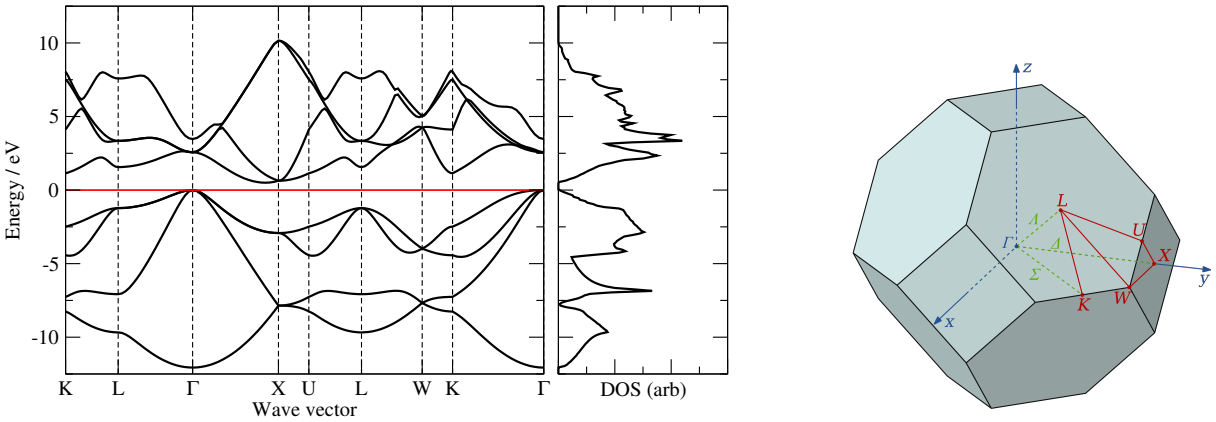

Figure 2: Properties of silicon. Left panel: electronic band structure and density of states (DOS). Right panel: first Brillouin zone (IBZ).

Fig. 2 shows the electronic band structure of silicon, containing 4 valence (*i.e.* occupied) and 4 conduction (*i.e.* empty) bands along several directions in the Brillouin zone (see right panel in Fig. 2 for the location of the high-symmetry points). The top of the valence band (in the case of silicon this is at the Γ point) is set as the zero of energy. As clearly visible from the figure,

an *energy band gap* separates occupied bands from empty bands (the experimental value of the band gap is about 1.1 eV).
Fig. 2 also illustrates the DOS of silicon. The DOS indicates how many electronic states are available at a specific value of the energy. Note that flat bands in the band-structure plot (i.e. bands whose energy does not significantly vary with the wavevector $\mathbf{k}$) correspond to sharp peaks in the DOS. For example, the band at $E \approx -7.5\,\text{eV}$ along the $U - L - W$ directions in the first Brillouin zone is almost dispertionless, corresponding to a very sharp peak in the DOS at this energy.

1. The electronic band structure and the DOS of aluminium and copper are presented in Fig. 3. Starting from the electronic configuration of the Al and Cu atoms, try to recognize which band structure refers to Al and which one refers to Cu. Match the DOSs with the corresponding band structures.

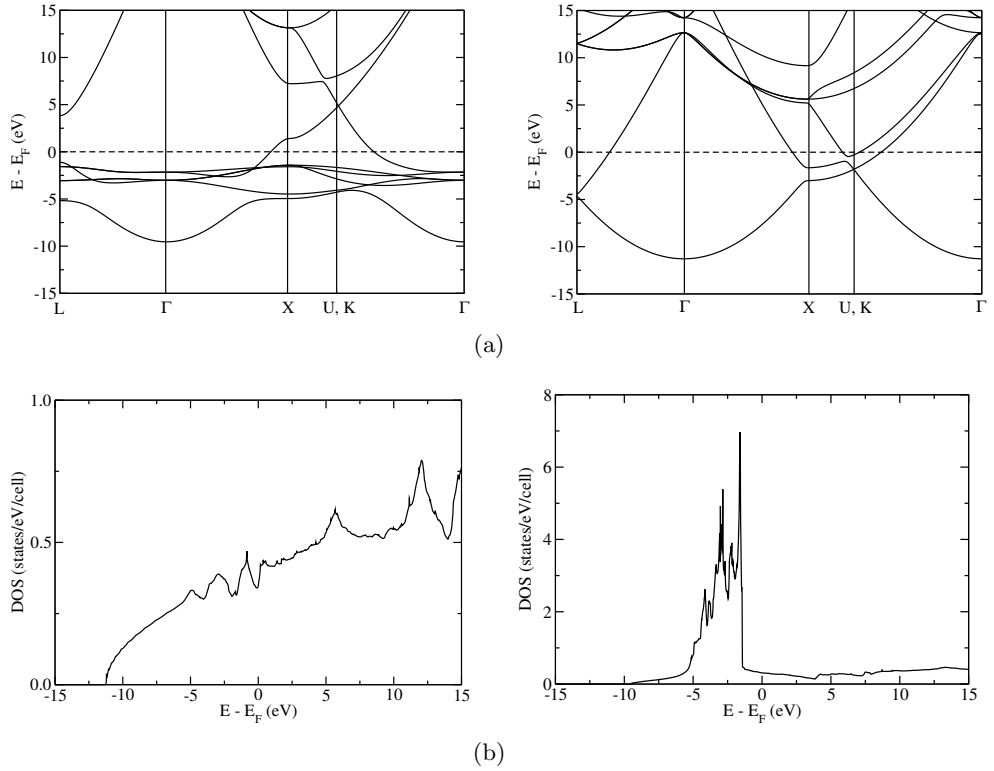

Figure 3: Electronic band structures (a) and density of states (DOS, b) for Al and Cu (in random order). E_F is the Fermi energy.

2. Consider the electronic band structures of three prototypical semiconductors, namely Ge, Si, and GaAs (see Fig. 4).

   Which of these semiconductors has a direct band gap and which one has an indirect band gap? Where are the top of the valence band and the bottom of the conduction band located?

   What is the wavelength of a photon whose energy equals the band gap of each material? From the wavelength, determine the momentum of the photon. How does it compare to the size of the first Brillouin zone for each material? Use the following lattice parameters:

for Ge $a = 5.66\,\text{Å}$, for Si $a = 5.43\,\text{Å}$, and for GaAs $a = 5.65\,\text{Å}$. Which of these materials will absorb the radiation with such a photon? Why?

(*Hint: In the absorption process, both energy and momentum should be conserved.*)

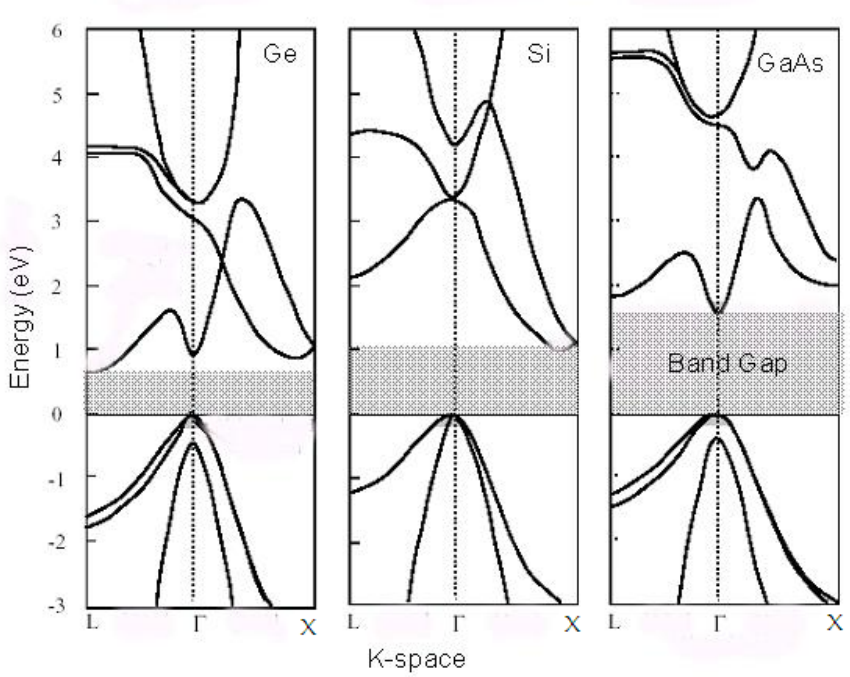

Figure 4: Electronic band structures of Ge, Si, and GaAs.