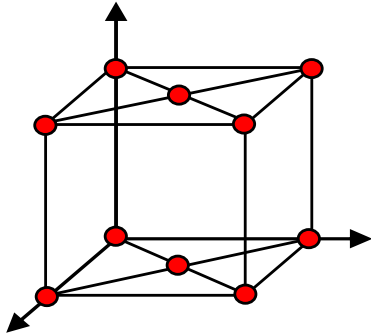


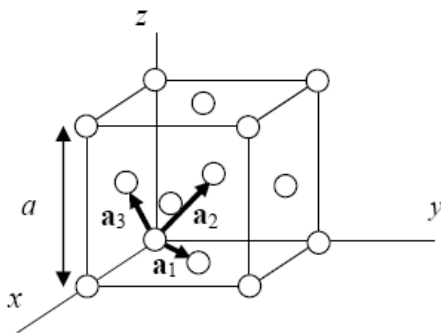
EXERCISES

CRYSTAL STRUCTURE

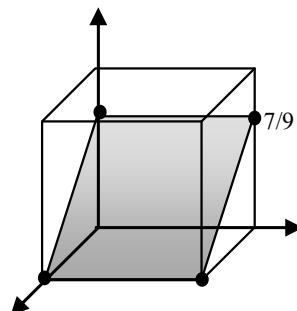
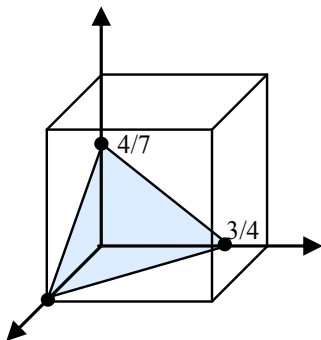
- Exemplify on the side-centered cubic lattice in the figure below the point group operations used to classify Bravais lattices.



- Draw the planes with Miller indices (100) and (001) with respect to the primitive translation vectors of the simple cubic lattice. What are the Miller indices of the same planes when referred to the primitive axes of the fcc lattice represented in the figure below?



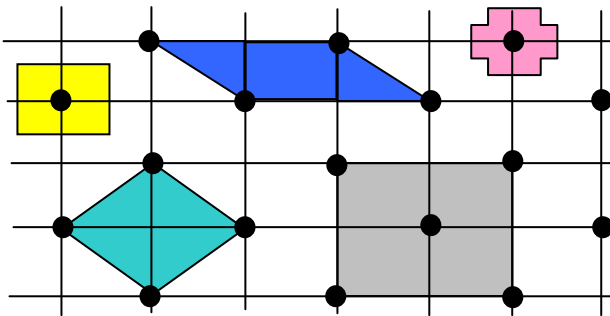
- Determine the Miller indices of the planes in the figures below.



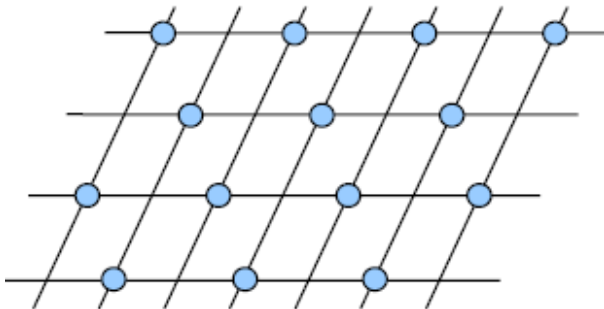
For a family of planes characterized by the Miller indices (mnp) that you have determined, find the distance between two planes in these families if the lattice is a simple cubic lattice and a face-centered cubic lattice. The general formulas are given below:

$$d_{mnp}^{sc} = \frac{a}{\sqrt{m^2 + n^2 + p^2}}, \quad d_{mnp}^{fcc} = \frac{a}{\sqrt{(n+p-m)^2 + (p+m-n)^2 + (m+n-p)^2}}$$

- Which of the cells in the figure below are primitive? Is there a Wigner-Seitz cell in the figure below or not?

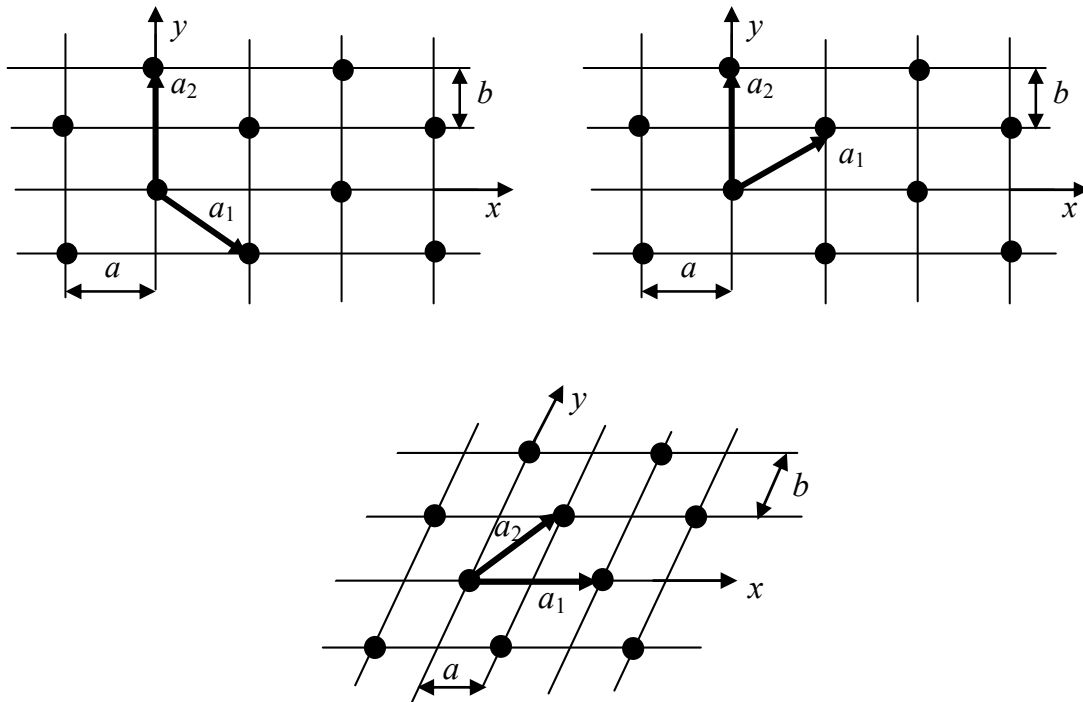


- Find the primitive cell, the Wigner-Seitz cell and the point group symmetries for the lattice in the figure below



RECIPROCAL LATTICE

- Using the orthogonality relation $\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}$ between the primitive translation vectors \mathbf{a}_i in the direct lattice and the vectors \mathbf{b}_i in the reciprocal lattice, find the reciprocal lattice of the direct lattices in the figures below. The Kronecker symbol is defined as: $\delta_{ij} = 1$ if $i = j$, and 0 otherwise.



- Construct the first Brillouin zone for the two-dimensional lattices in the figures above.

X-RAY DIFFRACTION

- Estimate the order of magnitude of the kinetic energy of neutrons that can be used in diffraction experiments to obtain the crystal structures. By assuming that the neutron beam arises from a gas, estimate the order of magnitude of the temperature required to have diffraction.

- Suppose that in a linear crystal with N lattice points at positions $\mathbf{R}_m = m\mathbf{a}$, where $m = 0, \dots, N-1$, identical scatterers with local electronic concentration n_{loc} are located at every lattice points. By analogy to the result in the course, show that the total radiation amplitude,

which in this case takes the expression $F = n_{loc} \sum_{m=0}^{N-1} \exp(-ima \cdot \Delta\mathbf{k})$, is equal to

$$F = n_{loc} \cdot \frac{1 - \exp(-iNa \cdot \Delta\mathbf{k})}{1 - \exp(-ia \cdot \Delta\mathbf{k})}.$$

Then, show that $|F|^2$ can be expressed as $|F|^2 = |n_{loc}|^2 \frac{\sin^2(N\mathbf{a} \cdot \Delta\mathbf{k} / 2)}{\sin^2(\mathbf{a} \cdot \Delta\mathbf{k} / 2)}$

(Hint: use the relations $\sum_{m=0}^{N-1} x^m = \frac{1-x^N}{1-x}$ and $\sin x = [\exp(ix) - \exp(-ix)] / 2i$.)

Demonstrate that the scattered intensity, proportional to $|F|^2$, takes maximum values when $\mathbf{a} \cdot \Delta\mathbf{k} = 2\pi s$, where s is an integer. If we change $\Delta\mathbf{k}$ slightly such that $\mathbf{a} \cdot \Delta\mathbf{k} = 2\pi s + \varepsilon$, where ε gives the position of the first zero in $\sin(N\mathbf{a} \cdot \Delta\mathbf{k} / 2)$, find the value ε and relate it to N . This result indicates that the width of the diffraction maximum becomes extremely narrow for macroscopic values of N .

- Starting from the definition of the structure factor, $S_G = \sum_{j=1}^s f_j \exp(-i\mathbf{G} \cdot \mathbf{r}_j)$, where f_j is the atomic form factor in an elementary cell with s atoms in the basis and \mathbf{G} is a vector in the reciprocal lattice, find the structure factor of a face-centered cubic lattice considered as a simple cubic lattice with four atoms per unit cell with coordinates $[[000]]$, $[[1/2, 1/2, 0]]$, $[[0, 1/2, 1/2]]$, and $[[1/2, 0, 1/2]]$. Consider that the atomic form factors of all the atoms in the cell are identical and use the following expressions for the primitive lattice vectors of the Bravais and the reciprocal lattice: $\mathbf{a}_1 = a\mathbf{x}$, $\mathbf{a}_2 = a\mathbf{y}$, $\mathbf{a}_3 = a\mathbf{z}$, and $\mathbf{b}_1 = (2\pi/a)\mathbf{x}$, $\mathbf{b}_2 = (2\pi/a)\mathbf{y}$, $\mathbf{b}_3 = (2\pi/a)\mathbf{z}$, respectively. Estimate the diffracted light intensity $I_{mnp} = |S_{mnp}|^2$ of the planes (110) and (100).

- For the hydrogen atom in its ground state, the electronic concentration has a radial dependence only given by $n(\rho) = (\pi a_B^3)^{-1} \exp(-2\rho/a_B)$, where a_B is the Bohr radius. Show that the atomic form factor, $f = \int n(\mathbf{r}) \exp(-i\mathbf{G} \cdot \mathbf{r}) dV = 4\pi \int_0^\infty n(\rho) \rho^2 (\sin G\rho / G\rho) d\rho$, is equal to $f(G) = 16 / (4 + G^2 a_B^2)^2$. Calculate the limits of the form factor when $G = 0$ and $G a_B \gg 1$.

- Consider a linear chain of different atoms ABAB..., where the distance between A and B is $a/2$. If f_A and f_B are the form factors of atoms A and B, respectively, and the incident X-ray beam is perpendicular to the line of atoms, show that a) the interference condition is $n\lambda = a \cos \theta$, with n an integer and θ the angle between the diffracted beam and the chain of atoms, and b) the intensity of the diffracted beam is proportional to $|f_A - f_B|^2$ for n odd and

$|f_A + f_B|^2$ for n even. What happens when $f_A = f_B$? What is the result when the distance between atoms A and B is different from $a/2$?

CRYSTAL BINDING

- For solid hydrogen, which crystallizes in a fcc structure, measurements indicate that the Lennard-Jones parameters are $\gamma = 5 \cdot 10^{-22}$ J and $\sigma = 2.96$ Å. If the energy of the crystal composed of N atoms is given by $U_{cryst} = 2N\gamma \left[S_{12} \left(\frac{\sigma}{R} \right)^{12} - S_6 \left(\frac{\sigma}{R} \right)^6 \right]$, find the cohesive energy per hydrogen atom for $S_{12} = 12.13$ and $S_6 = 14.45$. Which is the equilibrium distance between hydrogen atoms?

- Consider a line of $2N$ ions of alternating charge $\pm e$ with a repulsive potential energy A/R^n between nearest neighbors. Show that at equilibrium $U(R_0) = -\frac{2Ne^2 \ln 2}{R_0} \left(1 - \frac{1}{n} \right)$, where R_0 is the equilibrium distance.

PHONONS

- Consider a longitudinal wave $u_n(t) = u_0 \exp[i(kan - \omega t)]$ which propagates in a linear chain of identical atoms with mass M , spacing a and nearest-neighbor interaction A . Show that the total energy of the wave is

$$E = \frac{M}{2} \sum_n (du_n / dt)^2 + \frac{A}{2} \sum_n (u_n - u_{n+1})^2.$$

If the expression of u_n is substituted in the expression above, demonstrate that the total time-averaged energy per atom is

$$\frac{1}{4} M \omega^2 u_0^2 + \frac{1}{2} A [1 - \cos(ka)] u_0^2 = \frac{1}{2} M \omega^2 u_0^2,$$

where in the last step we have used the dispersion relation $\omega(k) = 2\sqrt{A/M} |\sin(ka/2)|$ for this problem.

- Consider the normal modes of a linear chain with atoms of the same mass M , in which the interatomic force between nearest-neighbor atoms are alternatively A and $10A$. If the nearest-neighbor separation is $a/2$, find the dispersion relation $\omega(k)$ and particularize it for $k = 0$ and $k = \pi/a$. This problem models a crystal of diatomic molecules, such as H_2 .

- Calculate the dispersion of phonons in an atomic chain taking into account the interactions with the second nearest neighbors, characterized by the interatomic force constant A_2 . In this case, the interaction with nearest neighbors is described by the interatomic force constant A_1 . Does this interaction modify the first Brillouin zone? Does it modify the group velocity values at the center and edges of the Brillouin zone?

- Consider a linear chain of ions of equal mass but alternating charge, the charge of the n th ion being $e_n = e(-1)^n$. In this case, besides the short-range interactions between nearest neighbors characterized by the interatomic force constant A , there is also a Coulomb interaction between all ions. Show that the dispersion relation in this case becomes

$$\omega^2 / \omega_0^2 - \sin^2(ka/2) + \gamma \sum_{n=1}^{\infty} (-1)^n [1 - \cos(nka)] / n^3,$$

where $\omega_0 = 2\sqrt{A/M}$, $\gamma = e^2 / Aa^3$.

ELECTRONS

- In a cubic crystal with lattice constant a , the \mathbf{k} -dependence of the electron energy is

$$E_{\mathbf{k}} = E_a - C - 2A[\cos(k_1a) + \cos(k_2a) + \cos(k_3a)]$$

where E_a , C and A are constant parameters. Derive the acceleration of an electron due to an external electric field.

Derive the dispersion relation in a coordinate system that is rotated in the \mathbf{k} space with $\pi/4$ with respect to the original system.

- For a one-dimensional crystal with lattice constant a , the dispersion relation is

$$E(k) = E_0 + E_1 \sin^2(ka/2)$$

with E_0 and E_1 constant parameters. Derive the effective mass and draw its dependence on the k vector. Find the values of the effective mass at the center and boundaries of the first Brillouin zone. What is the group velocity of electrons in this crystal?

- Same problem as above for a two-dimensional crystal with a dispersion relation

$$E_{\pm}(\mathbf{k}) = \pm t \sqrt{3 + 2 \cos(\sqrt{3}k_y a) + 4 \cos(\sqrt{3}k_y a / 2) \cos(3k_x a / 2)},$$

where a is the lattice constant and t is a parameter.

- Assuming that the electrons follow a Schrödinger equation with effective mass m , calculate the electronic density of states

a) in a two-dimensional lattice, in which electrons are free to propagate with effective mass m along the directions x and y , but are confined by infinite potential wells in the z directions, in a region of width L_z . Such a structure is called a quantum well.

b) in a one-dimensional lattice, in which electrons are free to propagate with effective mass m along the x direction, but are confined by infinite potential wells in the y and z directions, in region of respective widths L_y and L_z . This structure is called a quantum wire.

c) in a zero-dimensional lattice, in which electrons are confined by infinitely high potential barriers in a small spatial region with dimensions L_x , L_y and L_z . Assume that the effective electron mass is m . This structure is called a quantum dot.

In all cases the electron momentum along the directions of confinement can only take discrete values, which are derived imposing the condition of vanishing wavefunction at the infinite potential wells.