Estado Sólido I
Tarea 1: Estructura Cristalina

Dr. Omar De la Peña Seaman

20 enero 2025

Nombre del Estudiante: _____

Problema 1 *Properties of basic crystal structures*

(a) Calculate the first nearest-neighbor distance for the bcc and fcc crystal structures.

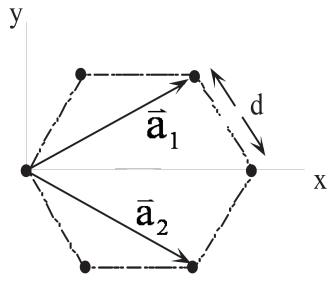
(b) Obtain the packing fraction f_e for the bcc and fcc crystal structures.

(c) Show that the c/a ratio for an ideal hexagonal close-packed structure is $(8/3)^{1/2} = 1.633$.

. . . . . .

Problema 2 *Graphene structure*

Graphene forms a two-dimensional honeycomb lattice with carbon atoms at the corners of a hexagon separated by a distance d. The primitive lattice vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ are shown in the figure.



(a) Find the lattice vector's magnitude $|\mathbf{a}_1|$ and $|\mathbf{a}_2|$ in terms of d, and call this magnitude a.

(b) Rewrite $\mathbf{a}_1$ and $\mathbf{a}_2$ in terms of a and express them in Cartesian coordinates with unit vectors $\hat{\mathbf{i}}$ and $\hat{\mathbf{j}}$.

(c) How many atoms does graphene have in the conventional and the primitive unit cells? Which are their positions? (in Cartesian coordinates).

. . . . . .

Problema 3 *Interplanar separation and Bragg condition*

Consider a diffraction event in a crystal lattice, where the distance between two adjacent parallel planes is d. Then:

(a) Show for a simple cubic lattice that $d^2 = a^2/(h^2 + k^2 + l^2)$.

(b) Show that the diffraction condition $2\mathbf{k} \cdot \mathbf{G} = G^2$ is an analogous statement of the Bragg condition, $2d\text{Sin}\theta = n\lambda$.

. . . . . .

Problema 4 *Direct and reciprocal lattices*

(a) Show that the reciprocal lattice of the reciprocal lattice is the original lattice again.

(b) Show that fcc and bcc lattice are reciprocal each other.

. . . . . .

Problema 5 *Structure factor of diamond*

Consider the diamond crystal structure as a conventional cubic cell with a basis of eight atoms if the cell, then:

(a) Find the structure factor S of this basis.

(b) Find the zeros of S and show that the allowed reflections of the diamond structure satisfy $v_1 + v_2 + v_3 = 4n$, where all indices are even and n is any integer, or else all indices are odd.

. . . . . .