Estado Sólido
Posgrado en Ciencias Físicas 2012-2
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TAREA 2
Fecha de entrega: 23 de febrero 2012 antes de la clase

Problema 1

4. (a) Prove that the Wigner-Seitz cell for any two-dimensional Bravais lattice is either a hexagon or a rectangle.

(b) Show that the ratio of the lengths of the diagonals of each parallelogram face of the Wigner-Seitz cell for the face-centered cubic lattice (Figure 4.16) is $\sqrt{2}$:1.

(c) Show that every edge of the polyhedron bounding the Wigner-Seitz cell of the body-centered cubic lattice (Figure 4.15) is $\sqrt{2}/4$ times the length of the conventional cubic cell.

(d) Prove that the hexagonal faces of the bcc Wigner-Seitz cell are all regular hexagons. (Note that the axis perpendicular to a hexagonal face passing through its center has only threefold symmetry, so this symmetry alone is not enough.)

Problema 2

6. The face-centered cubic is the most dense and the simple cubic is the least dense of the three cubic Bravais lattices. The diamond structure is less dense than any of these. One measure of this is that the coordination numbers are: fcc, 12; bcc, 8; sc, 6; diamond, 4. Another is the following: Suppose identical solid spheres are distributed through space in such a way that their centers lie on the points of each of these four structures, and spheres on neighboring points just touch, without overlapping. (Such an arrangement of spheres is called a close-packing arrangement.) Assuming that the spheres have unit density, show that the density of a set of close-packed spheres on each of the four structures (the "packing fraction") is:

$$
\begin{aligned}
&\text{fcc:} && \sqrt{2}\pi/6 = 0.74\\
&\text{bcc:} && \sqrt{3}\pi/8 = 0.68\\
&\text{sc:} && \pi/6 = 0.52\\
&\text{diamond:} && \sqrt{3}\pi/16 = 0.34.
\end{aligned}
$$

Problema 3

1. (a) Prove that the reciprocal lattice primitive vectors defined in (5.3) satisfy

$$\mathbf{b}_1 \cdot (\mathbf{b}_2 \times \mathbf{b}_3) = \frac{(2\pi)^3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}. \tag{5.15}$$

(*Hint:* Write $\mathbf{b}_1$ (but not $\mathbf{b}_2$ or $\mathbf{b}_3$) in terms of the $\mathbf{a}_i$, and use the orthogonality relations (5.4).)

(b) Suppose primitive vectors are constructed from the $\mathbf{b}_i$ in the same manner (Eq. (5.3)) as the $\mathbf{b}_i$ are constructed from the $\mathbf{a}_i$. Prove that these vectors are just the $\mathbf{a}_i$ themselves; i.e., show that

$$2\pi \frac{\mathbf{b}_2 \times \mathbf{b}_3}{\mathbf{b}_1 \cdot (\mathbf{b}_2 \times \mathbf{b}_3)} = \mathbf{a}_1, \quad \text{etc.} \tag{5.16}$$

(*Hint:* Write $\mathbf{b}_3$ in the numerator (but not $\mathbf{b}_2$) in terms of the $\mathbf{a}_i$, use the vector identity $\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = \mathbf{B}(\mathbf{A} \cdot \mathbf{C}) - \mathbf{C}(\mathbf{A} \cdot \mathbf{B})$, and appeal to the orthogonality relations (5.4) and the result (5.15) above.)

(c) Prove that the volume of a Bravais lattice primitive cell is

$$v = |\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)|, \tag{5.17}$$

where the $\mathbf{a}_i$ are three primitive vectors. (In conjunction with (5.15) this establishes that the volume of the reciprocal lattice primitive cell is $(2\pi)^3/v$.)

Problemas 4 y 5

2. (a) Using the primitive vectors given in Eq. (4.9) and the construction (5.3) (or by any other method) show that the reciprocal of the simple hexagonal Bravais lattice is also simple hexagonal, with lattice constants $2\pi/c$ and $4\pi/\sqrt{3}a$, rotated through 30° about the c-axis with respect to the direct lattice.

(b) For what value of c/a does the ratio have the same value in both direct and reciprocal lattices? If c/a is ideal in the direct lattice, what is its value in the reciprocal lattice?

(c) The Bravais lattice generated by three primitive vectors of equal length a, making equal angles θ with one another, is known as the trigonal Bravais lattice (see Chapter 7). Show that the reciprocal of a trigonal Bravais lattice is also trigonal, with an angle θ^* given by $-\cos\theta^* = \cos\theta/[1 + \cos\theta]$, and a primitive vector length a^*, given by $a^* = (2\pi/a)(1 + 2\cos\theta\cos\theta^*)^{-1/2}$.

3. (a) Show that the density of lattice points (per unit area) in a lattice plane is d/v, where v is the primitive cell volume and d the spacing between neighboring planes in the family to which the given plane belongs.

(b) Prove that the lattice planes with the greatest densities of points are the $\{111\}$ planes in a face-centered cubic Bravais lattice and the $\{110\}$ planes in a body-centered cubic Bravais lattice. (*Hint:* This is most easily done by exploiting the relation between families of lattice planes and reciprocal lattice vectors.)