

Solid State Physics Homework 1

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Solution

(a) Consider Figure 1. Suppose there are N points in an area A on a certain lattice plane. The volume between A and its counterpart on an adjacent lattice plane is

$$V_{\text{total}} = Ad$$

Now since there are N points in A , there are N primitive unit cells between A and its counterpart, so

$$V_{\text{total}} = NV.$$

Thus

$$NV = Ad, \quad \text{areal density} := \frac{N}{A} = \frac{d}{V}. \quad (1)$$

(b) To maximize the areal density of lattice points is to maximize d .

Solution Below I use the side length of the so-called cubes as the length unit.

(a) Based-centered cubic is a Bravais lattice but the name is not on the list of 14. It is not really cubic, because it doesn't have the rotational symmetry around the x and y axes. It's actually a simple tetragonal lattice with $a = 1/\sqrt{2}$, $c = 1$, and the primitive vectors are

$$\mathbf{a}_1 = (1/2, -1/2, 0), \quad \mathbf{a}_2 = (1/2, 1/2, 0), \quad \mathbf{a}_3 = (0, 0, 1). \quad (2)$$

(b) Similar to the first case, side-centered cubic is also a Bravais lattice but not cubic, because it also doesn't have the rotational symmetry around the x and y axes and therefore is not really "cubic". It's actually a body-centered tetragonal lattice with $a = 1/\sqrt{2}$, $c = 1$. The primitive vectors are the same with (2).

(c) The edge-centered cubic lattice has the symmetry of a cube and therefore has to be a cubic lattice. By counting the number of lattice points, we find Figure 2 shows one unit cell. No translation symmetry is able to turn one of the points into another, so the unit cell is actually a primitive one. Thus the edge-centered cubic lattice is actually a simple cubic lattice: in each primitive unit cell, there are four points. So the edge-centered cubic lattice is not a Bravais lattice. It's the simple cubic lattice plus the basis shown as black (or red, or blue) in Figure 2.

Solution In each conventional cell of the bcc lattice, there are 2 lattice points, and so is the case for hcp. The volume of a conventional cell of the bcc lattice is a^3 . In the hcp lattice, $c = 2\sqrt{6}a/3$, so the volume is

$$\frac{\sqrt{3}}{2}a^2 \times c = \sqrt{2}a^3.$$

So to keep the density invariant,

$$\sqrt{2}a_{\text{hcp}}^3 = a_{\text{bcc}}^3,$$

and

$$a_{\text{hcp}} = 2^{-1/6}a_{\text{bcc}} = 3.77 \text{ \AA}. \quad (3)$$

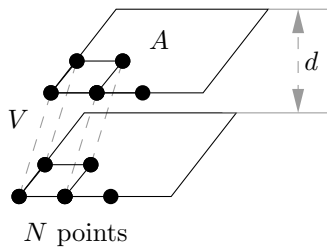


Figure 1: The volume between two areas on adjacent lattice planes

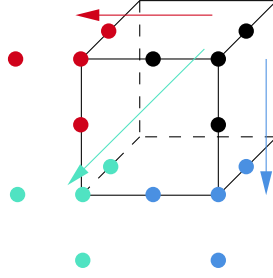


Figure 2: One unit cell of a edge centered cubic lattice

Solution

(a) There is only one Ti atom in the cube given, and obviously it's impossible to use a translation symmetry operation to turn one atom into another in the cube. The lattice is a simple cubic lattice, and the primitive lattice vectors are

$$\mathbf{a}_1 = (1, 0, 0), \quad \mathbf{a}_2 = (0, 1, 0), \quad \mathbf{a}_3 = (0, 0, 1). \quad (4)$$

(b) There are five: $1/4 \times 4 = 1$ Sr atom, 1 Ti atom, and $1/2 \times 6 = 3$ O atoms. The coordinates of the Ti atom are $(1/2, 1/2, 1/2)$. The coordinates of the Sr atom are $(0, 0, 0)$. The coordinates of the O atoms are $(1/2, 1/2, 0)$, $(0, 1/2, 1/2)$, $(1/2, 0, 1/2)$.

(c) The nearest neighbors of a Sr atom are 12 Ti atoms. The nearest neighbors of a Ti atom are 6 O atoms. The nearest neighbors of an O atom are 2 Ti atoms.