9.2. Layer stacking

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9.2.1. Layer stacking in close-packed structures (By D. Pandey and P. Krishna)

The crystal structures of a large number of materials can be described in terms of stacking of layers of atoms. This chapter provides a brief account of layer stacking in materials with structures based on the geometrical principle of close packing of equal spheres.

9.2.1.1. *Close packing of equal spheres*

9.2.1.1.1. *Close-packed layer*

In a close-packed layer of spheres, each sphere is in contact with six other spheres as shown in Fig. 9.2.1.1. This is the highest number of nearest neighbours for a layer of identical spheres and therefore yields the highest packing density. A single close-packed layer of spheres has two-, three- and sixfold axes of rotation normal to its plane. This is depicted in Fig. 9.2.1.2(*a*), where the size of the spheres is reduced for clarity. There are three symmetry planes with indices $(1\bar{2}.0)$, $(\bar{2}1.0)$, and (11.0) defined with respect to the smallest two-dimensional hexagonal unit cell shown in Fig. 9.2.1.2(*b*). The point-group symmetry of this layer is $6mm$ and it has a hexagonal lattice. As such, a layer with such an arrangement of spheres is often called a hexagonal close-packed layer. We shall designate the positions of spheres in the layer shown in Fig. 9.2.1.1 by the letter '*A*'. This *A* layer has two types of triangular interstices, one with the apex angle up (△) and the other with the apex angle down (▽). All interstices of one kind are related by the same hexagonal lattice as that for the *A* layer. Let the positions of layers with centres of spheres above the centres of the △ and ▽ interstices be designated as '*B*' and '*C*', respectively. In the cell of the *A* layer shown in Fig. 9.2.1.1 ($a = b =$ diameter of the sphere and $\gamma = 120°$), the three positions *A*, *B*, and *C* on projection have coordinates $(0, 0)$, $(\frac{1}{3}, \frac{2}{3})$, and $(\frac{2}{3}, \frac{1}{3})$, respectively.

9.2.1.1.2. *Close-packed structures*

A three-dimensional close-packed structure results from stacking the hexagonal close-packed layers in the *A*, *B*, or *C* position with the restriction that no two successive layers are in identical positions. Thus, any sequence of the letters *A*, *B*, and *C*, with no two successive letters alike, represents a possible manner of stacking the hexagonal close-packed layers. There are thus infinite possibilities for close-packed layer stackings. The identity period n of these layer stackings is determined by the number of layers after which the stacking sequence starts repeating itself. Since there are two possible positions for a new layer on the top of the preceding layer, the total number of possible layer stackings with a repeat period of n is 2^{n-1}.

In all the close-packed layer stackings, each sphere is surrounded by 12 other spheres. However, it is touched by all 12 spheres only if the axial ratio h/a is $\sqrt{2/3}$, where h is the separation between two close-packed layers and a is the diameter of the spheres (Verma & Krishna, 1966). Deviations from the ideal value of the axial ratio are common, especially in hexagonal metals (Cottrell, 1967). The arrangement of spheres described above provides the highest packing density of 0.7405 in the ideal case for an infinite lattice (Azaroff, 1960). There are, however, other arrangements of a finite number of equal spheres that have a higher packing density (Boerdijk, 1952).

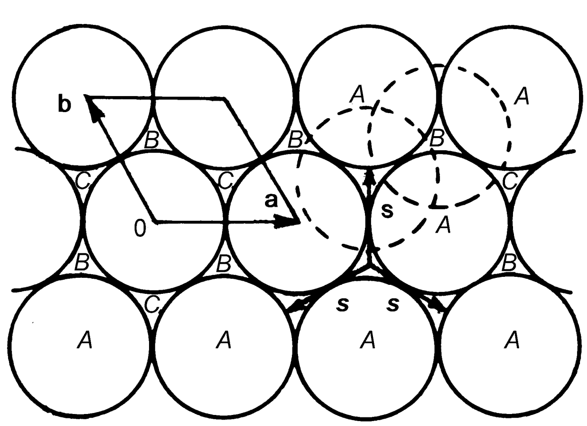

Fig. 9.2.1.1. The close packing of equal spheres in a plane.

9.2.1.1.3. *Notations for close-packed structures*

In the Ramsdell notation, close-packed structures are designated as nX, where n is the identity period and X stands for the lattice type, which, as shown later, can be hexagonal (H), rhombohedral (R), or in one special case cubic (C) (Ramsdell, 1947).

In the Zhdanov notation, use is made of the stacking offset vector $\mathbf{s}$ and its opposite $-\mathbf{s}$, which cause, respectively, a

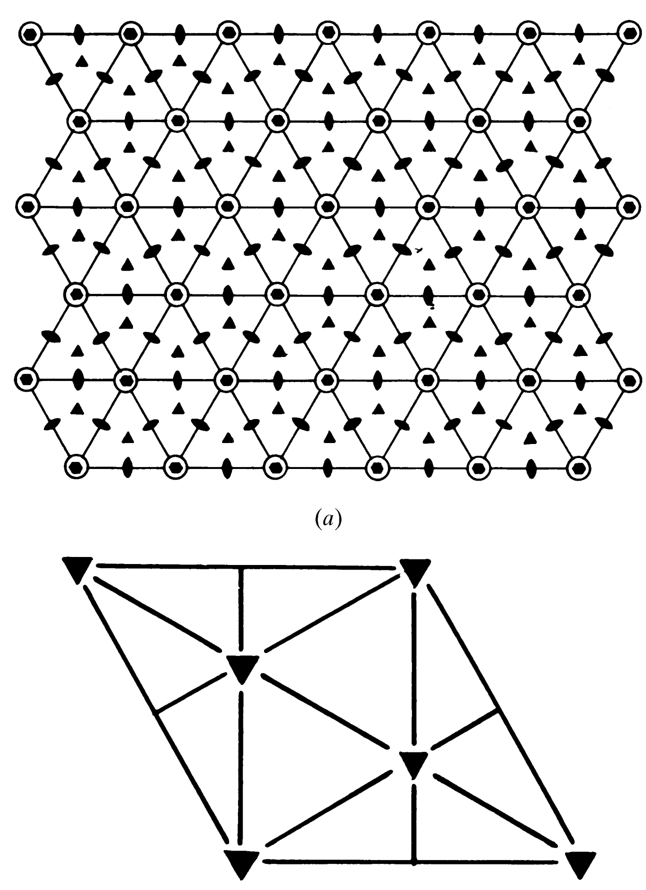

Fig. 9.2.1.2. (*a*) Symmetry axes of a single close-packed layer of spheres and (*b*) the minimum symmetry of a three-dimensional close packing of spheres.

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