9.2. LAYER STACKING

Table 9.2.1.1. *Common close-packed metallic structures*

Stacking sequence	Identity period	Ramsdell notation	Zhdanov notation	Jagodzinski notation	Proto-type
$AB, A \ldots$	2	$2H$	11	h	Mg
$ABC, A \ldots$	3	$3C$	∞	c	Cu
$ABCB, A \ldots$	4	$4H$	22	hc	La
$ABCBCACAB, A \ldots$	9	$9R$	21	hhc	Sm

cyclic $(A \to B \to C \to A)$ or anticyclic $(A \to C \to B \to A)$ shift of layers in the same plane. The vector **s** can be either $(1/3)[1\bar{1}00]$, $(1/3)[01\bar{1}0]$, or $(1/3)[\bar{1}010]$. Zhdanov (1945) suggested summing the number of consecutive offsets of each kind and designating them by numeral figures. Successive numbers in the Zhdanov symbol have opposite signs. The rhombohedral stackings have three identical sets of Zhdanov symbols in an identity period. It is usually sufficient to write only one set.

Yet another notation advanced, amongst others, by Jagodzinski (1949*a*) makes use of configurational symbols for each layer. A layer is designated by the symbol *h* or *c* according as its neighbouring layers are alike or different. Letter '*k*' in place of '*c*' is also used in the literature.

Some of the common close-packed structures observed in metals are listed in Table 9.2.1.1 in terms of all the notations.

9.2.1.2. *Structure of compounds based on close-packed layer stackings*

Frequently, the positions of one kind of atom or ion in inorganic compounds, such as SiC, ZnS, CdI_2, and GaSe, correspond approximately to those of equal spheres in a close packing, with the other atoms being distributed in the voids. All such structures will also be referred to as close-packed structures though they may not be ideally close packed. In the close-packed compounds, the size and coordination number of the smaller atom/ion may require that its close-packed neighbours in the neighbouring layers do not touch each other.
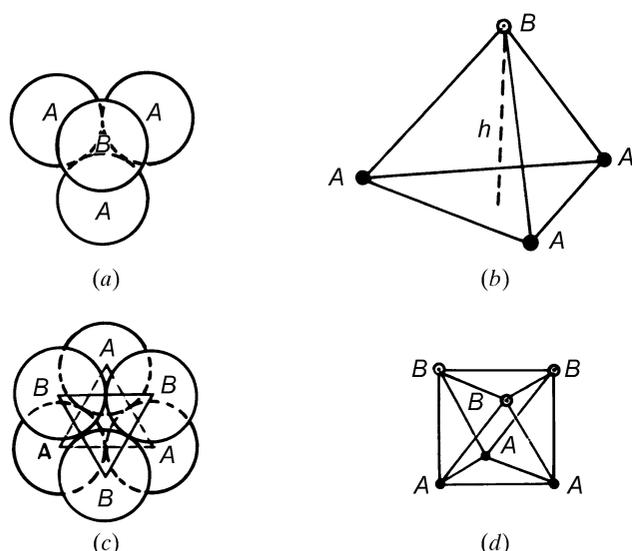
9.2.1.2.1. *Voids in close packing*

Three-dimensional close packings of spheres have two kinds of voids (Azaroff, 1960):

(i) If the triangular interstices in a close-packed layer have spheres directly over them, the resulting voids are called tetrahedral voids because the four spheres surrounding the void are arranged at the corners of a regular tetrahedron (Figs. 9.2.1.3*a*,*b*). If R denotes the radius of the four spheres surrounding a tetrahedral void, the radius of the sphere that would just fit into this void is given by $0.225R$ (Verma & Krishna, 1966). The centre of the tetrahedral void is located at a distance $3h/4$ from the centre of the sphere on top of it.

(ii) If the triangular interstices pointing up in one close-packed layer are covered by triangular interstices pointing down in the adjacent layer, the resulting voids are called octahedral voids (Figs. 9.2.1.3*c*,*d*) since the six spheres surrounding each such void lie at the corners of a regular octahedron. The radius of the sphere that would just fit into an octahedral void is given by $0.414R$ (Verma & Krishna, 1966). The centre of this void is located half way between the two layers of spheres.

While there are twice as many tetrahedral voids as the spheres in close packing, the number of octahedral voids is equal to the number of spheres (Krishna & Pandey, 1981).

9.2.1.2.2. *Structures of SiC and ZnS*

SiC has a binary tetrahedral structure in which Si and C layers are stacked alternately, each carbon layer occupying half the tetrahedral voids between successive close-packed silicon layers. One can regard the structure as consisting of two identical interpenetrating close packings, one of Si and the other of C, with the latter displaced relative to the former along the stacking axis through one fourth of the layer spacing. Since the positions of C atoms are fixed relative to the positions of layers of Si atoms, it is customary to use the letters A, B, and C as representing Si–C double layers in the close packing. To be more exact, the three kinds of layers need to be written as $A\alpha$, $B\beta$, and $C\gamma$ where Roman and Greek letters denote the positions of Si and C atoms, respectively. Fig. 9.2.1.4 depicts the structure of SiC-6*H*, which is the most common modification.
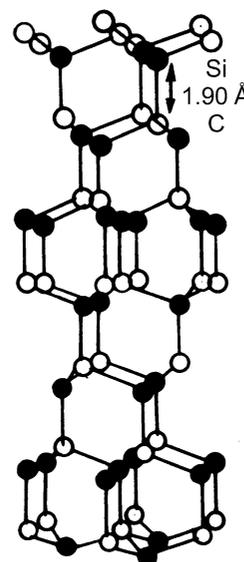

(*a*) (*b*)

(*c*) (*d*)

Fig. 9.2.1.3. Voids in a close packing: (*a*) tetrahedral void; (*b*) tetrahedron formed by the centres of spheres; (*c*) octahedral void; (*d*) octahedron formed by the centres of spheres.

Fig. 9.2.1.4. Tetrahedral arrangement of Si and C atoms in the SiC-6*H* structure.

references