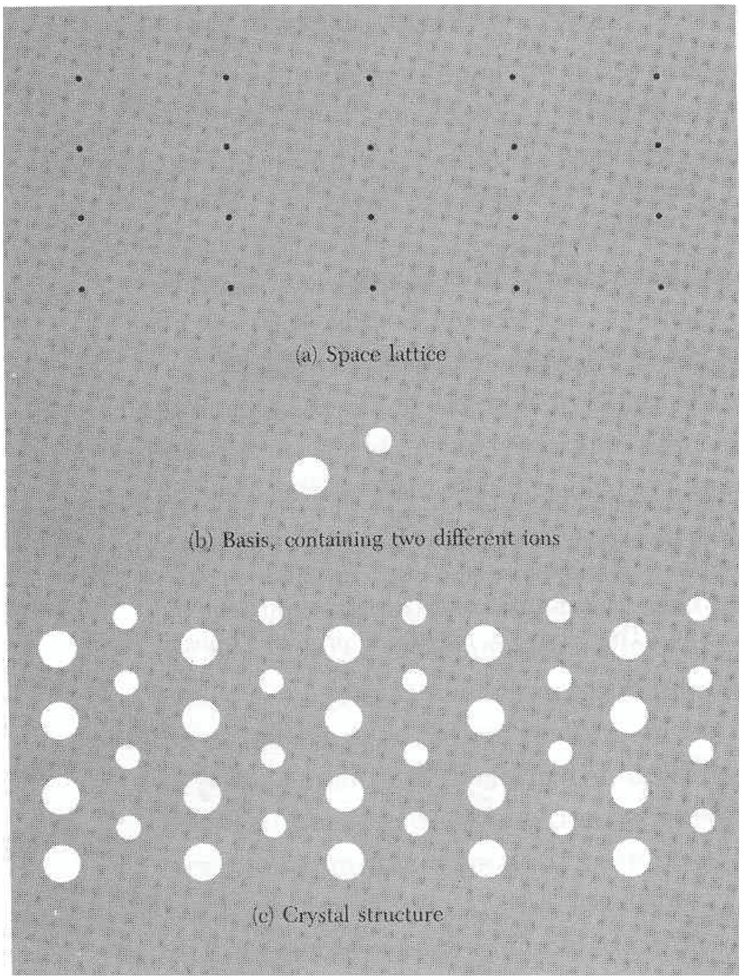
A Bravais lattice is a lattice in which every lattice points has exactly the same environment.

Bravais lattice

Basis (基元)

crystal structure



Bravais lattice + basis = crystal structure

A Bravais lattice can be spanned by primitive vectors.

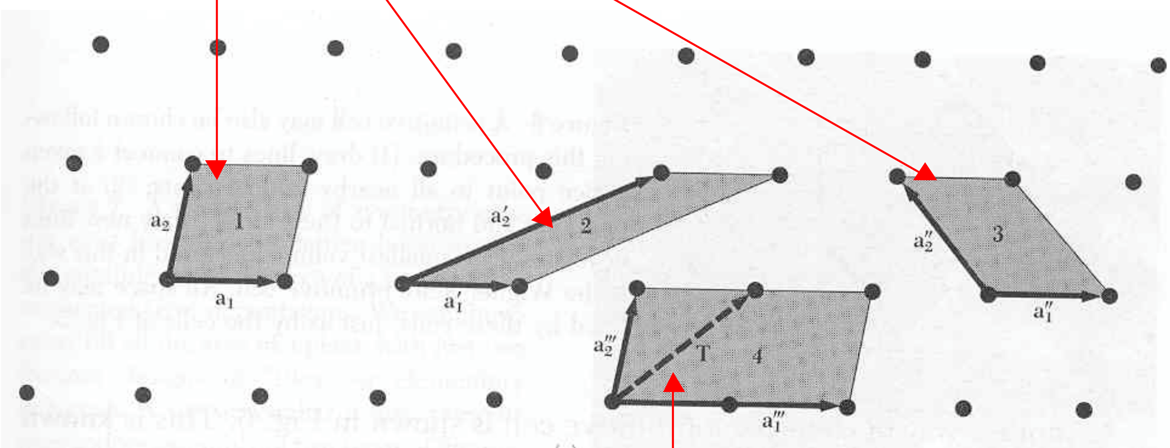
Lattice point $\mathbf{r} = n_1\mathbf{a_1}+n_2\mathbf{a_2}+n_3\mathbf{a_3}$

where n_1, n_2, and n_2 span ALL integers, and

$\mathbf{a_1}$, $\mathbf{a_2}$, and $\mathbf{a_3}$ are primitive vectors

For example, in 2-dm,

primitive unit cell (原始晶胞)

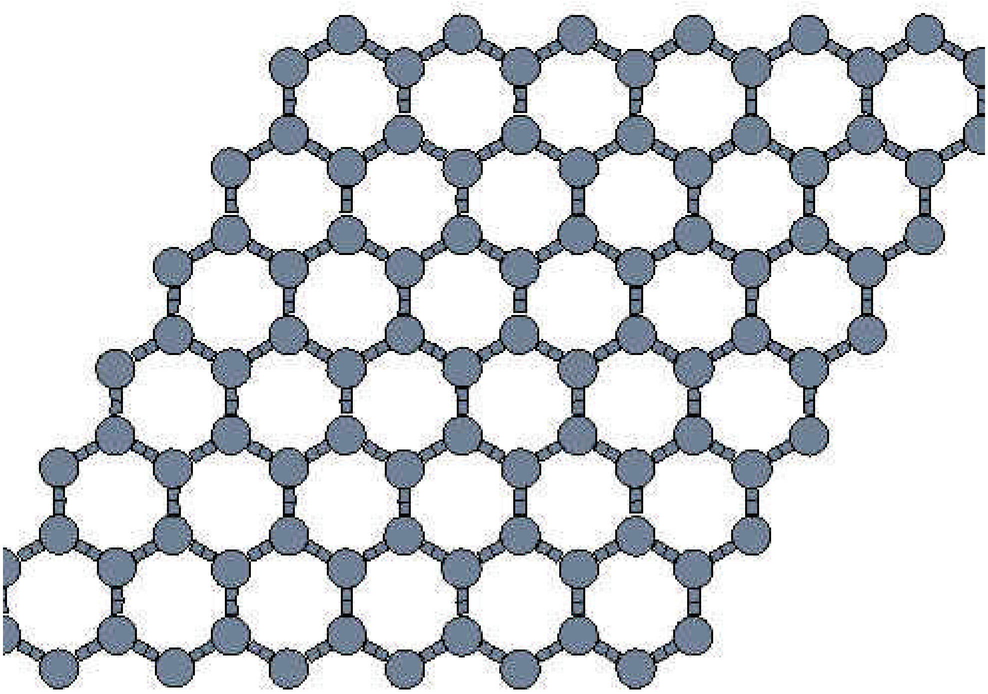


nonprimitive unit cell

one primitive unit cell contains one lattice point

An example: graphite (honeycomb lattice)

- Is it a Bravais lattice (where no "basis" is needed)?
- Find out the primitive vectors and basis (if exists).

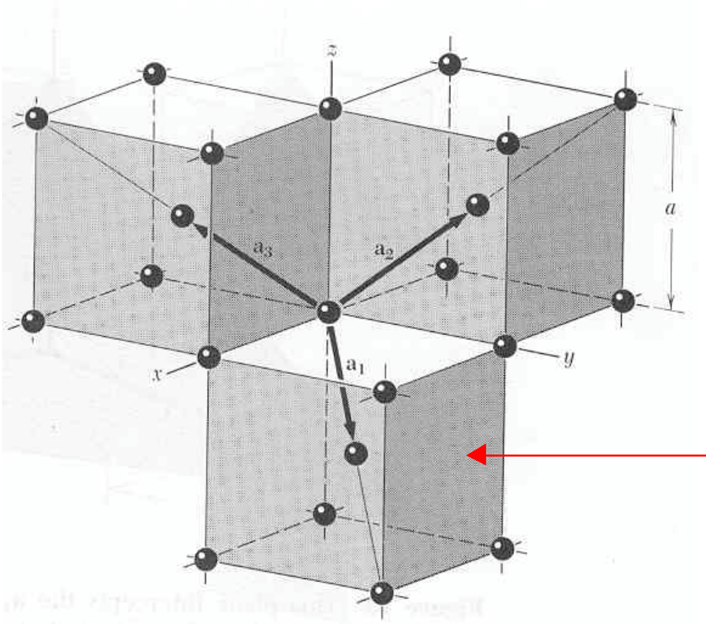


a honeycomb lattice = a triangular lattice + 2-point basis

3-dim crystal structures you need to know

(some are simple Bravais lattices, some are not)

1). bcc lattice (Li, Na, K, Rb, Cs… etc)



A conventional unit cell (nonprimitive)

primitive vectors

$$\vec{a}_1 = \frac{a}{2}(\ \ \hat{x}+\hat{y}-\hat{z}),$$

$$\vec{a}_1 = \frac{a}{2}(-\hat{x}+\hat{y}+\hat{z}),$$

$$\vec{a}_1 = \frac{a}{2}(\ \ \hat{x}-\hat{y}+\hat{z}).$$

Note: A bcc lattice is a Bravais lattice without a basis.

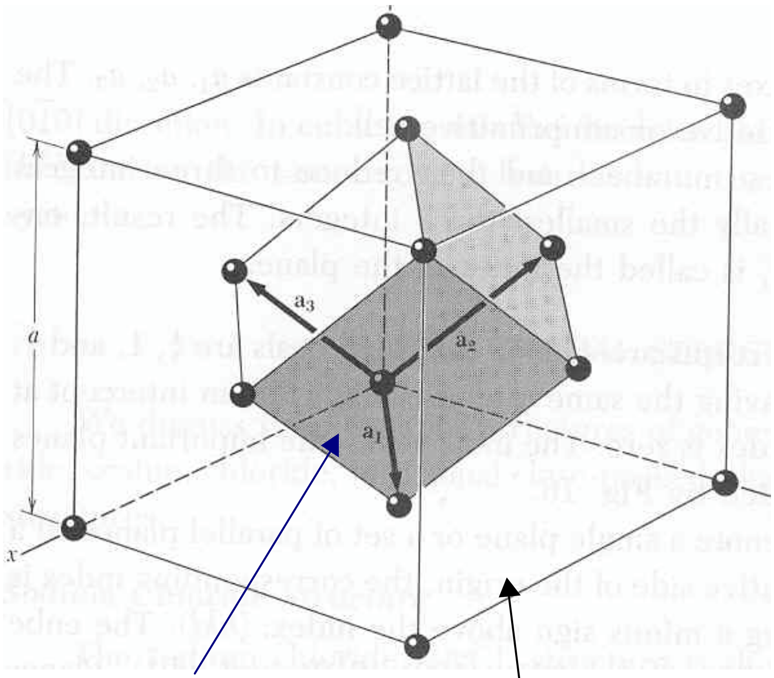
But we can also treat it as a cubic Bravais lattice with a 2-point basis! (to take advantage of the cubic symmetry.)

2). fcc lattice (Ne, Ar, Kr, Xe,

Al, Cu, Ag, Au… etc)

lattice

constant



a primitive unit cell

a conventional unit cell

primitive vectors

$$\vec{a}_1 = \frac{a}{2}(\hat{x}+\hat{y}),$$

$$\vec{a}_1 = \frac{a}{2}(\hat{y}+\hat{z}),$$

$$\vec{a}_1 = \frac{a}{2}(\hat{z}+\hat{x}).$$

a fcc lattice is also a Bravais lattice

3). hcp structure (= simple hexagonal lattice+ a 2-point basis.)

e.g. Be, Mg… etc.

2 overlapping “simple hexagonal lattices”

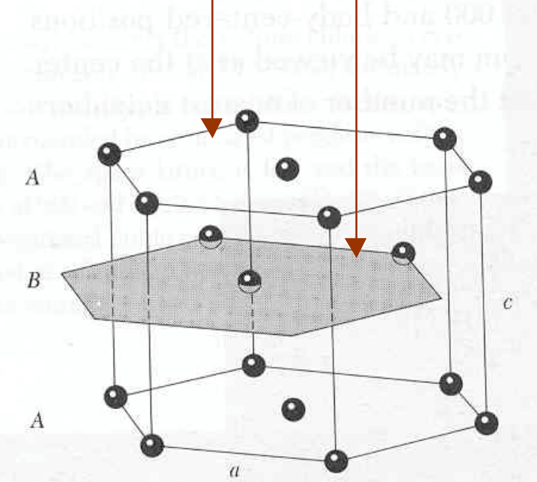


Figure 22 The hexagonal close-packed structure. The atom positions in this structure do not constitute a space lattice. The space lattice is simple hexagonal with a basis of two identical atoms associated with each lattice point. The lattice parameters a and c are indicated, where a is in the basal plane and c is the magnitude of the axis $\mathbf{a}_3$ of Fig. 14.

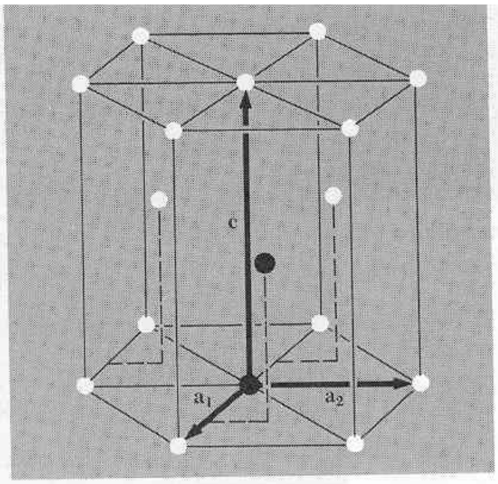
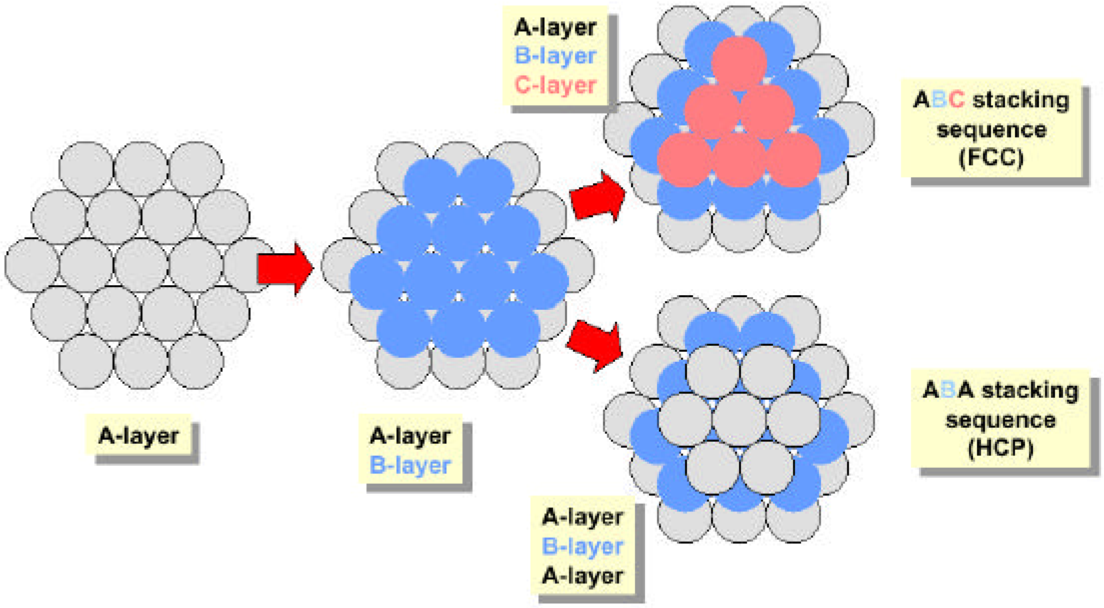


Figure 23 The primitive cell has $a_1 = a_2$, with an included angle of 120°. The c axis (or $\mathbf{a}_3$) is normal to the plane of $\mathbf{a}_1$ and $\mathbf{a}_2$. The ideal hcp structure has $c = 1.633\ a$. The two atoms of one basis are shown as solid circles. One atom of the basis is at the origin; the other atom is at $\frac{2}{3}\frac{1}{3}\frac{1}{2}$, which means at the position $\mathbf{r} = \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$.

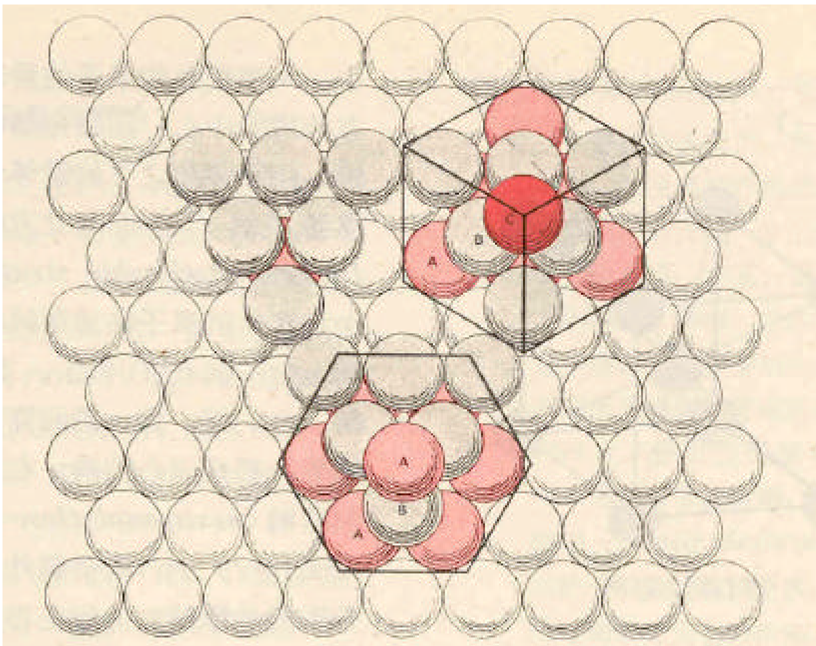
- Primitive vectors: $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{c}$
- The 2 atoms of the basis are located at the origin and

  at $r = (2/3)\ \mathbf{a}_1 + (1/3)\ \mathbf{a}_2 + (1/2)\mathbf{c}$
- ABABAB… stacking

The tightest way to pack spheres:



ABCABC…= fcc, ABAB…= hcp!



packing fraction = 74%, coordination number (配位數) = 12

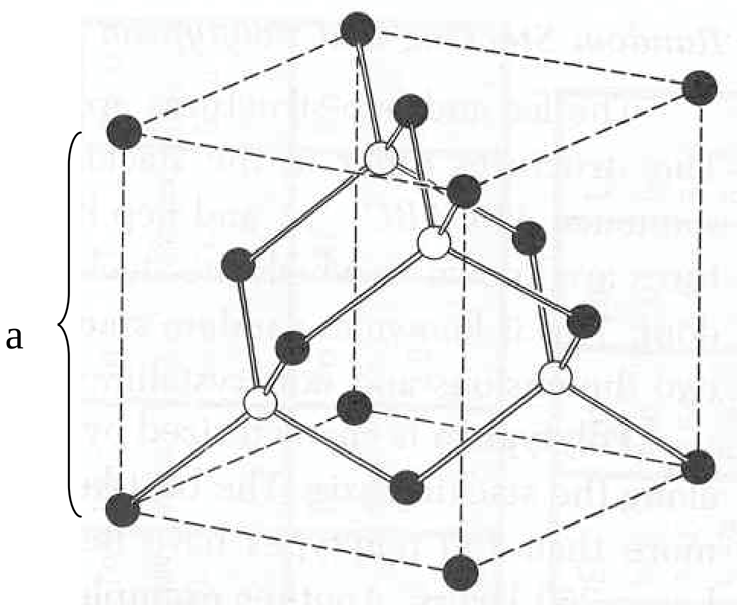
(Cf: bcc, packing fraction = 68%, coordination number = 8)

other close packed structures, ABABCAB… etc.

4). Diamond structure (C, Si, Ge… etc)

= fcc lattice + a 2-atom basis, $\mathbf{r}_1=\mathbf{0}$, $\mathbf{r}_2=(a/4)(\mathbf{x}+\mathbf{y}+\mathbf{z})$

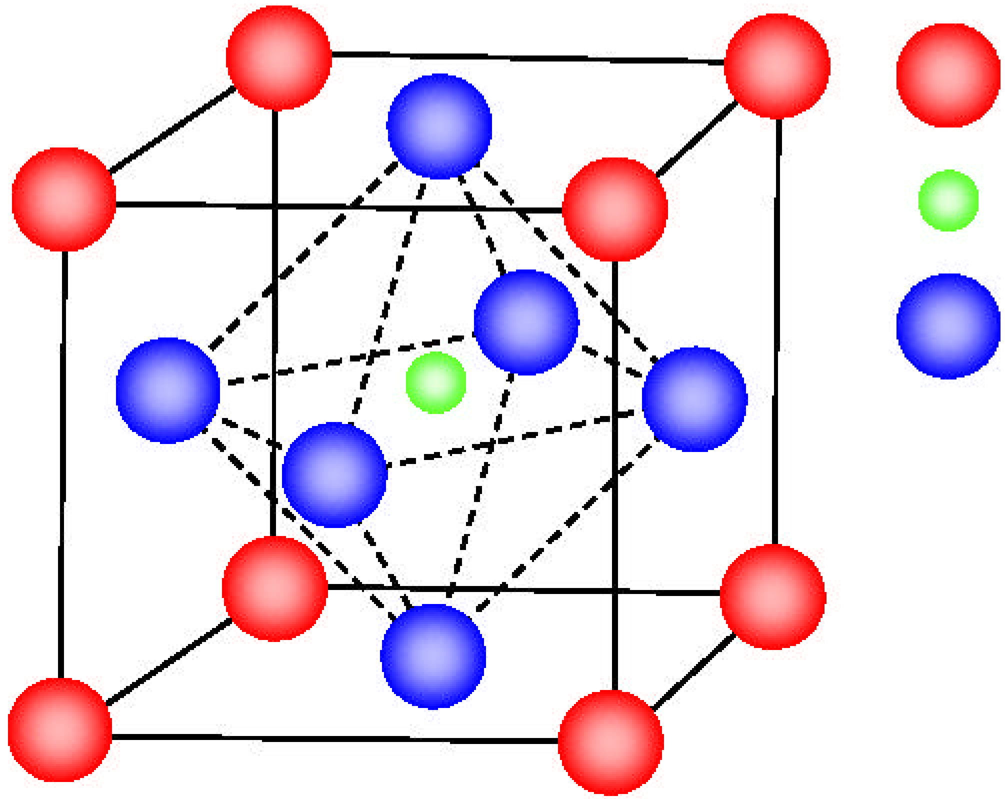
= 2 overlapping fcc lattices (one is displaced along the main diagonal by 1/4 distance)



- Low packing fraction (= 36% !)
- If the atoms in the basis are different, then it is called a Zincblend (閃鋅) structure (eg. GaAs, ZnS… etc).

  It is a familiar structure with an unfamiliar name.

Perovskite Type Structure ABO_3



A - cation: cubic lattice

B - cation: body centered

O - anion: face centered

oxidation state		examples
II / IV	A^{2+} / B^{4+}	$BaTiO_3$
		$Pb(Zr,Ti)O_3$
I / V	A^{+} / B^{5+}	$KTaO_3$
III / III	A^{3+} / B^{3+}	$LaMnO_3$

application: nonlinear resistors (PTC), SMD-capacitors, piezoelectric sensors and actuators, pyro-detectors, ferroelectric memory

Wigner-Seitz cell

The WS cell enclosing a lattice point is the region of space that is closer to that lattice point than to any other lattice point.

Method of construction:

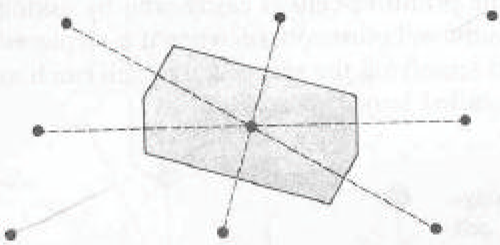
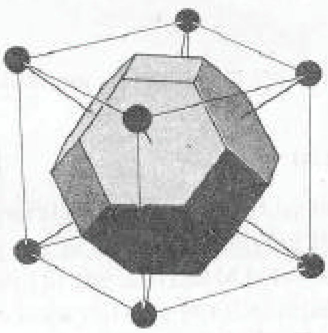


Figure 4.14
The Wigner-Seitz cell for a two-dimensional Bravais lattice. The six sides of the cell bisect the lines joining the central points to its six nearest neighboring points (shown as dashed lines). In two dimensions the Wigner-Seitz cell is always a hexagon unless the lattice is rectangular (see Problem 4a).

Figure 4.15
The Wigner-Seitz cell for the body-centered cubic Bravais lattice (a "truncated octahedron"). The surrounding cube is a conventional body-centered cubic cell with a lattice point at its center and on each vertex. The hexagonal faces bisect the lines joining the central point to the points on the vertices (drawn as solid lines). The square faces bisect the lines joining the central point to the central points in each of the six neighboring cubic cells (not drawn). The hexagons are regular (see Problem 4d).



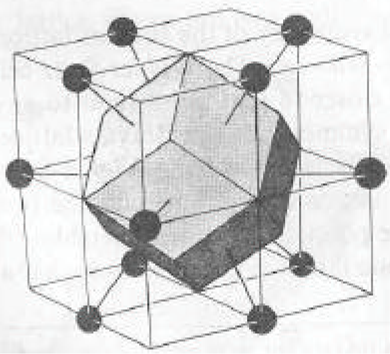


Figure 4.16
Wigner-Seitz cell for the face-centered cubic Bravais lattice (a "rhombic dodecahedron"). The surrounding cube is *not* the conventional cubic cell of Figure 4.12, but one in which lattice points are at the center of the cube and at the center of the 12 edges. Each of the 12 (congruent) faces is perpendicular to a line joining the central point to a point on the center of an edge.

advantage of using the WS cell:

same symmetry as the Bravais lattice

Miller indices (h,k,l) for crystal planes (see chap 5)

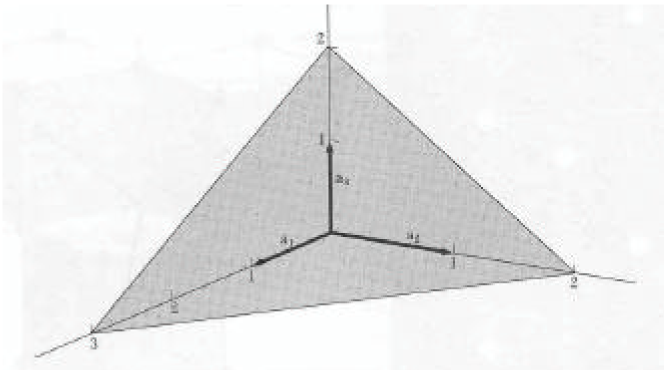


Figure 15 This plane intercepts the $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ axes at $3\mathbf{a}_1$, $2\mathbf{a}_2$, $2\mathbf{a}_3$. The reciprocals of these numbers are $\frac{1}{3}$, $\frac{1}{2}$, $\frac{1}{2}$. The smallest three integers having the same ratio are 2, 3, 3, and thus the indices of the plane are (233).

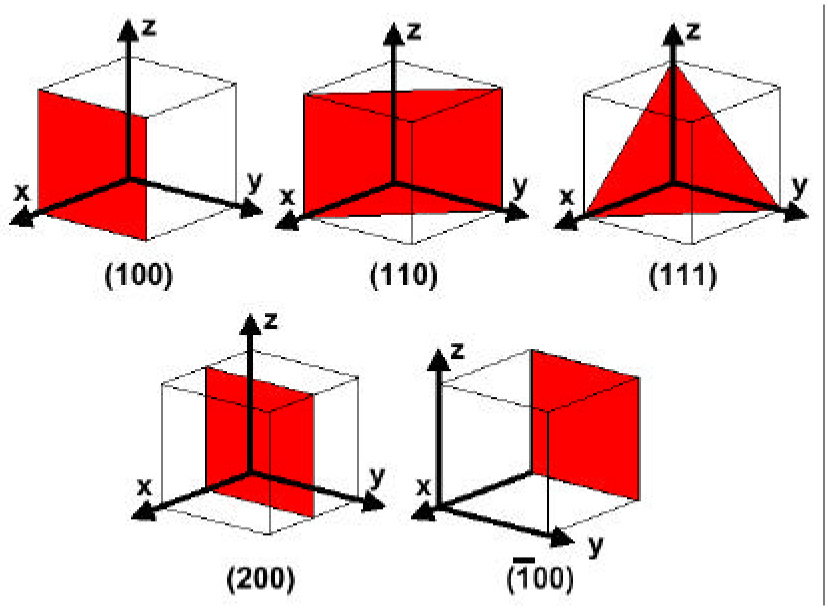
don’t need to be primitive

rules: 1. **取截距** (**以 $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ 為單位**) **得** (x, y, z)

2. **取倒數** (1/x,1/y,1/z)

3. **通分成互質整數** (h,k,l)

For example, cubic crystals (including bcc, fcc… etc)

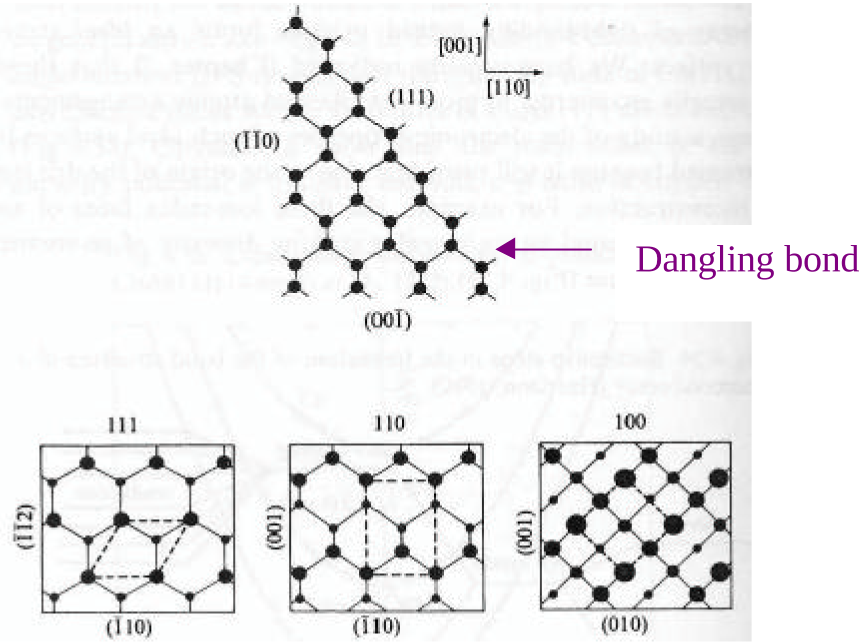


Note: Square bracket [h,k,l] refers to

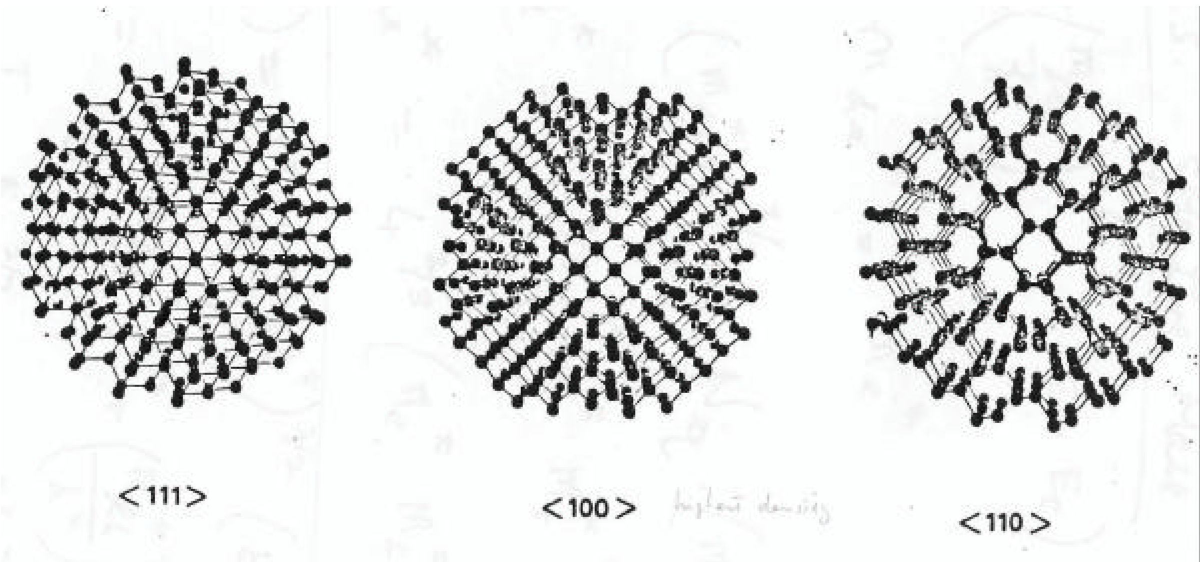
the “direction” $x\mathbf{a}_1+y\mathbf{a}_2+z\mathbf{a}_3$, instead of a crystal plane!

Diamond structure (eg. C, Si or Ge)

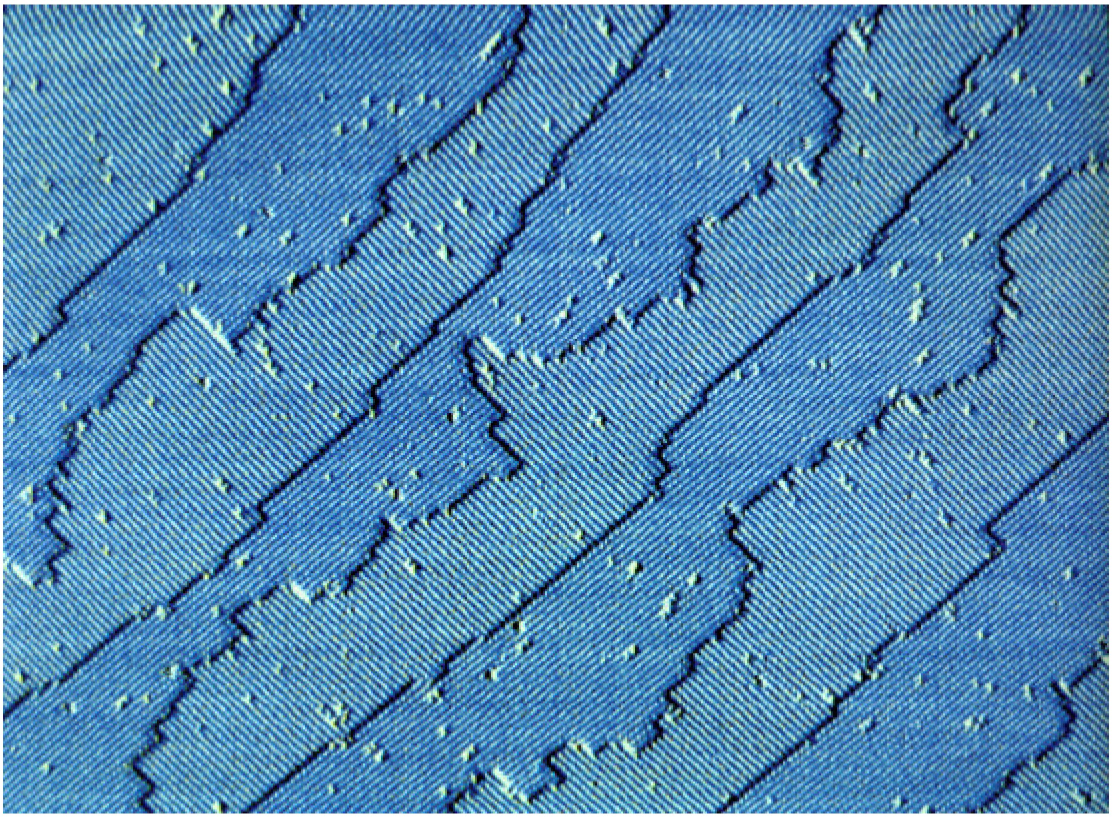
Termination of 3 low-index surfaces



lowest bond density (natural cleavage plane)



Actual Si(001) surface under STM (Kariotis and Lagally, 1991)



surface reconstruction (**重構**)

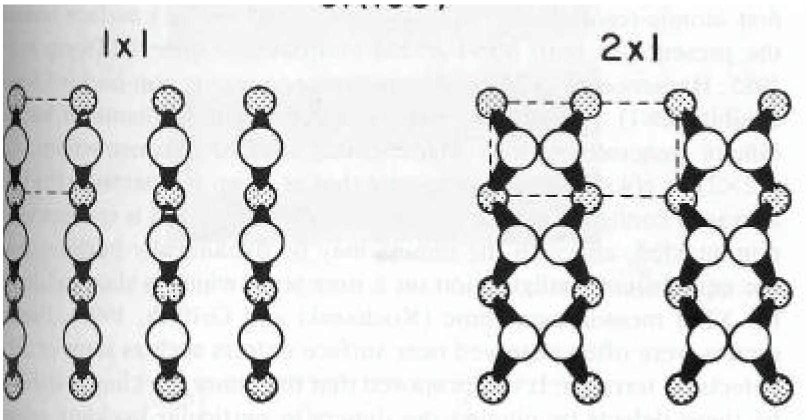
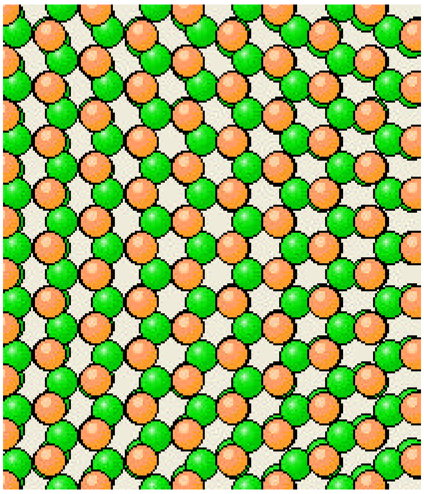


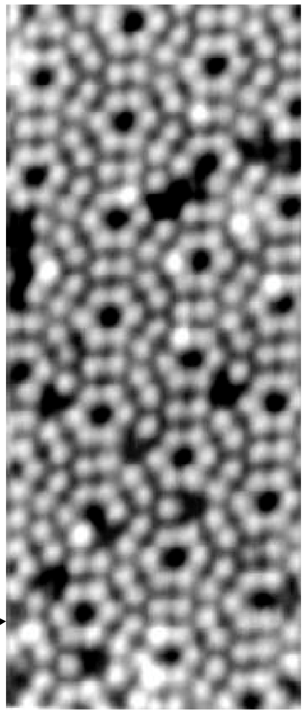
Fig. 4.16. Structural model for the Si(001) 2×1 surface.

Surface reconstruction on Si (111)

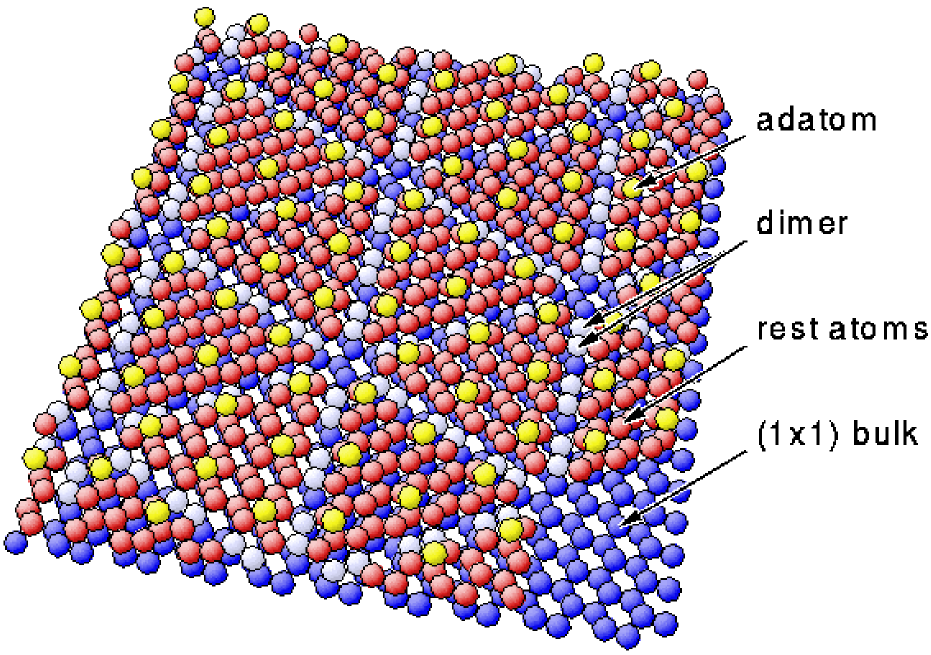
Si(111) un-reconstructed



STM image →



Detailed atom configuration



Si(111)-(7x7) DAS model (Takayanagi/Tong)

BALSAC plot