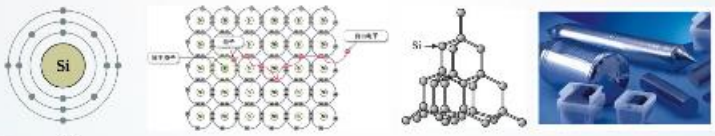
化学结构



C
Si
Ge
Sn

微观尺度 ⟹ 宏观尺度

电子 / 中子 ⟹ 离子 ⇧ 原子 ⇩ 分子 ⟹ 结合方式：金属键 / 共价键 / 离子键 / 范德华力 ⟹ 非晶 / 多晶 / 单晶

Ionization potential and electron affinity

电离势　　原子中移去一个电子所需的最小能量

- **Ionization potential**: the energy required to **remove** the most weakly bound (outermost) electron from an atom is known as the ionization potential (IP).

Absorb energy (IP)

Neutral Atom ⟹ Cationic Ion ($Atom^+$) + Free electron

亲和能　　原子获得一个电子形成负离子所放出的能量

- **Electron affinity**: the energy released when an **extra electron** is **attached** to an atom to form an anion is called the electron affinity (EA) of the atom.

Release energy (EA)

Neutral Atom + Free electron ⟹ Anionic ion ($Atom^-$)

- The higher IP means the harder to loss electron; the higher EA means the easier to gain extra electron

Different type of chemical bonding in solids

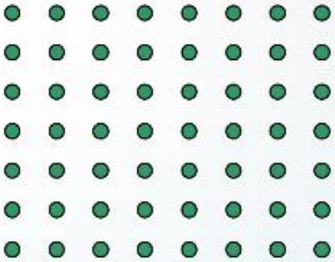
- General concept of cohesion and chemical bonding
- Ionic bonds
- Covalent bonds
- Metallic bonds
- Van der Waals bonds
- Hydrogen bonds

Si、Ge

AsGa 化合

2D lattice (二维晶格、点阵)

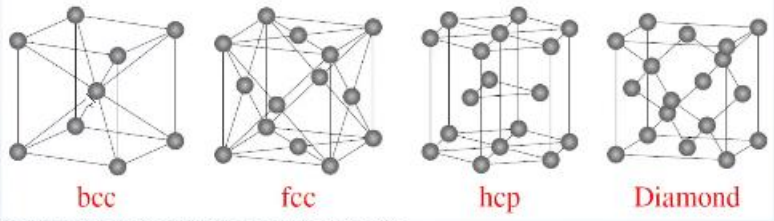
Periodicity or Repetition!



Definition of lattice

- periodic array (周期阵列) of atoms or group of atoms
- a structure unit infinitively extended, no boundary (边界) and interface (界面)

Crystal lattices commonly found in nature



bcc fcc hcp Diamond

body-centered cubic face-centered cubic

CN=8 CN=12 CN=12 CN=4

Mathematical description of lattices

--- Specify the location of a point in the lattice by r

--- Then the same point of any equivalent basis is described by

$$r' = r + u_1 a_1 + u_2 a_2 + u_3 a_3$$

u_1, u_2, u_3 are integers

--- Let u_1, u_2, u_3 run over any combination, we get lattice (note, not crystal structure)

Translation vector

The translational symmetry of lattice can be described by a lattice translation operation using translation vector （平移矢量）：

$$T(u_1, u_2, u_3) = u_1\mathbf{a}_1 + u_2\mathbf{a}_2 + u_3\mathbf{a}_3$$

Any two lattice points are connected by the T vector.

The special translational vectors (平移矢量):

$T(1, 0, 0) = \mathbf{a}_1$

$T(0, 1, 0) = \mathbf{a}_2$

$T(0, 0, 1) = \mathbf{a}_3$

are called "primitive translation vectors" （初基平移矢量）

Crystal Structure = Lattice + Basis

An ideal crystal is constructed by the infinite repetition of identical structural units in space. In the simplest crystals, the structural unit is a single atom, as in copper, iron, aluminum, etc. However, the smallest structural unit is NOT necessarily single atom, instead it can be a group of atoms or a molecule.

晶体结构的描述：基元+点阵
点阵：点在空间的周期排列

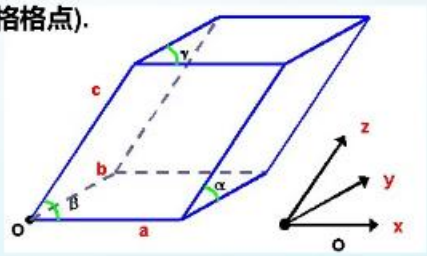
The structure of all crystals can be described in terms of a lattice, with a group of atoms attached to every lattice point. The group of atoms is called the basis; when repeated in space it forms the crystal structure.

UNIT CELL (晶胞)

The crystal structure of a material is often discussed in terms of its unit cell (晶胞). The unit cell is a tiny box containing one or more motifs, a spatial arrangement of atoms. The units cells are tiled in three-dimensional space to describe the crystal. The unit cell is given by its lattice parameters (晶格参数), the length of the cell edges and the angles between them, while the positions of the atoms inside the unit cell are described by the set of atomic positions (x_i,y_i,z_i) measured from a lattice point (晶格格点).

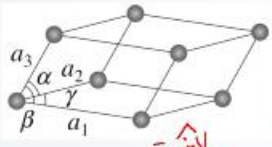
Unit cell is a box with:

- 3 sides - a, b, c
- 3 angles - α, β, γ

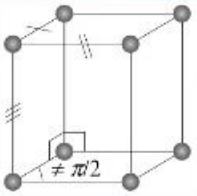


14

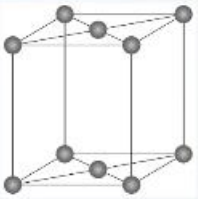
Fourteen Bravais Lattices



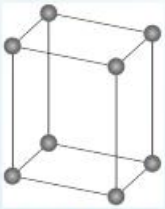
(Simple) Triclinic



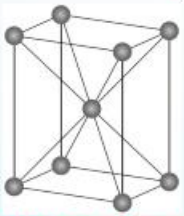
(Simple) Monoclinic



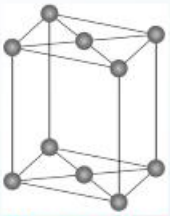
(Base-centered) Monoclinic



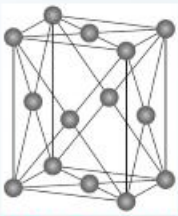
(Simple) Orthorhombic



(Body-centered) Orthorhombic

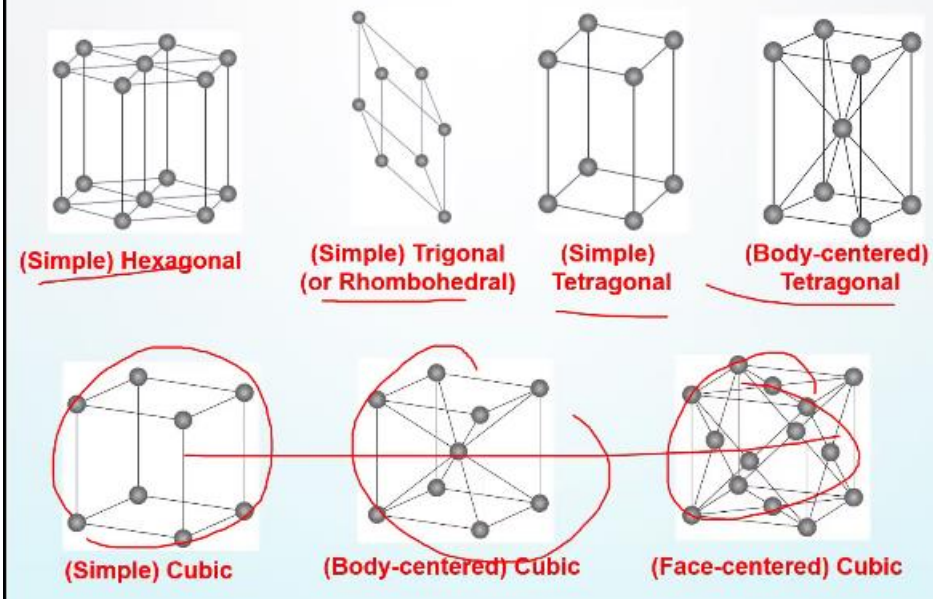


(Base-centered) Orthorhombic



(Face-centered) Orthorhombic

Fourteen Bravais Lattices



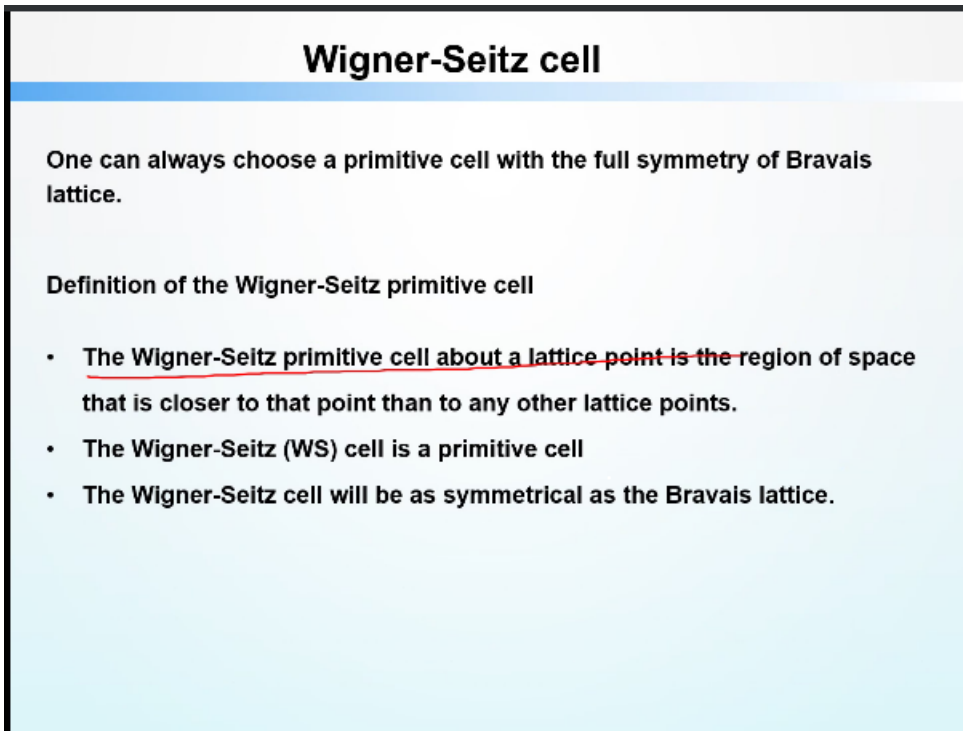
元胞不一定满足正交关系

Primitive unit cell（原胞）

A primitive cell (初基元胞), is a minimum cell corresponding to a single lattice point of a structure with translational symmetry in 2D or 3D. A lattice can be characterized by the geometry of its primitive cell.

A crystal can be categorized by its lattice and the atoms that lie in a primitive cell (the basis). A cell will fill all the lattice space without leaving gaps by repetition of crystal translation operations.

The volume, V_c, of the primitive cell is given by the primitive translation vectors $V_c = |\vec{a}_1 \bullet \vec{a}_2 \times \vec{a}_3|$



类似布里渊区方法（中垂线）

晶面指数，晶向指数