Introduction to Solid State Physics

Instructor: 張明哲

Textbook: *Introduction to Solid State Physics*, the 8ᵗʰ ed., by C. Kittel (1916-2019)

Grading: homework (40%), midterm exam (30%), final exam (30%)

TA: 朱彥儒

Required background: Fourier analysis, quantum physics

References:

• *The Oxford Solid State Basics, by S.H. Simon*

• *Solid State Physics, by H. Ibach and H. Lüth, the 4ᵗʰ ed.*

• *Solid State Physics, by N. Ashcroft and D. Mermin* (graduate level, but very good!)

Chap 1 Crystal structure

Chap 2 Wave diffraction and the reciprocal lattice

Chap 3 Crystal binding and elastic constants

Chap 4 Phonons I. Crystal vibrations

Chap 5 Phonons II. Thermal properties

Chap 6 Free-electron Fermi gas

Chap 7 Energy bands

Chap 9 Fermi surface and metals

Chap 8 Semiconductor crystals

The scope of solid state physics
Solid state physics studies physical properties of materials

Material	Structure	Shape	Properties
metal	crystal	bulk	mechanical
semiconductor	amorphous 非晶質	surface	thermal
insulator	quasicrystal準晶	interface	electrical
superconductor	… etc	nanocluster	magnetic
magnetic		… etc	optical
… etc			… etc

Solid state physics = {A} × {B} × {C} × {D} × …

Always try to understand a physical phenomenon from the microscopic point of view (atoms plus electrons)!

Chap 1   Crystal structure

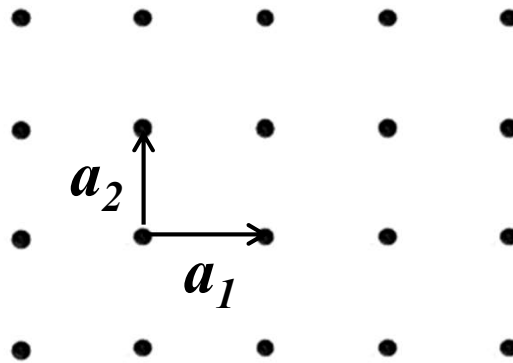salt on matrix © Smithsonian Institution

Dept of Phys

M.C. Chang

- A primitive lattice (in 3D) = a set of points with positions at

  $r = n_1 a_1 + n_2 a_2 + n_3 a_3$ (n_1, n_2, n_3 cover *all* integers),

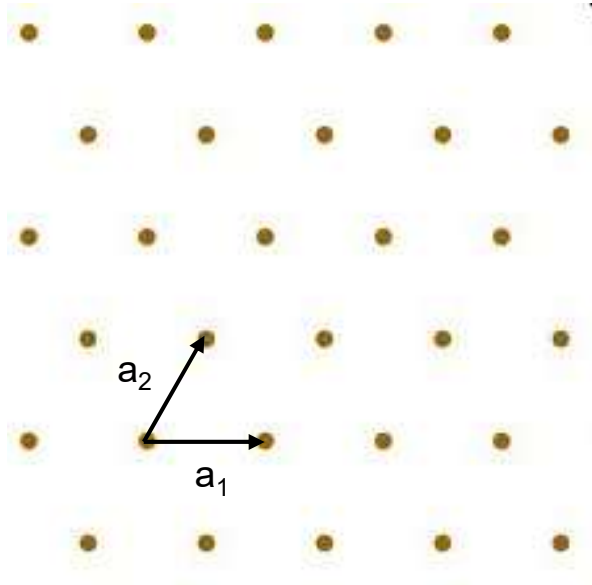 a_1, a_2, and a_3 are called primitive (translation) vectors 原始向量

Alternative definition:

- A primitive lattice = a set of points in which every point has

  exactly the same environment.

Note: A primitive lattice is often called a Bravais lattice.

From now on we'll use the latter term (*not* used by Kittel).

Bravais lattice

non-Bravais lattice
= Bravais lattice + basis 基元

For example,

Triangular (or hexagonal) lattice

Honeycomb lattice

a_2

a_1

Primitive vectors
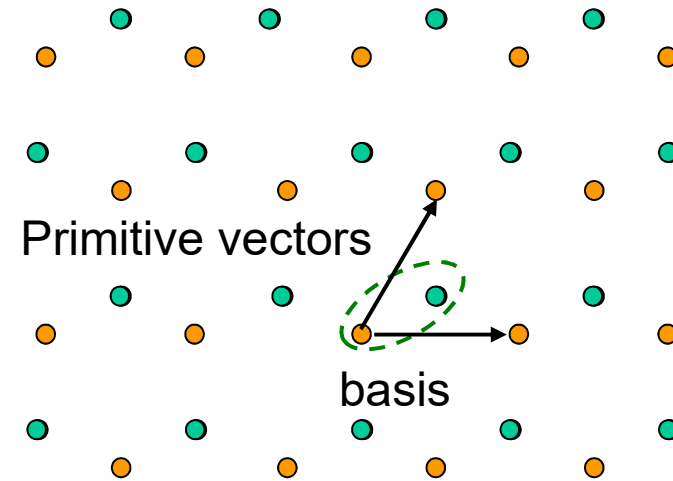
basis

Honeycomb lattice =

triangular lattice + 2-point basis

(i.e. overlap of 2 triangular lattices)

A simple way to determine the number of basis points:

Just look around from different atoms and see how many
different kinds of environment there are.

Crystal structure = Bravais lattice + basis of atoms

(How to repeat)   (What to repeat)
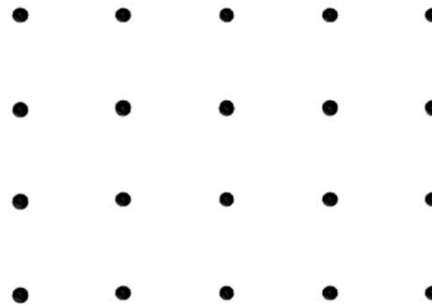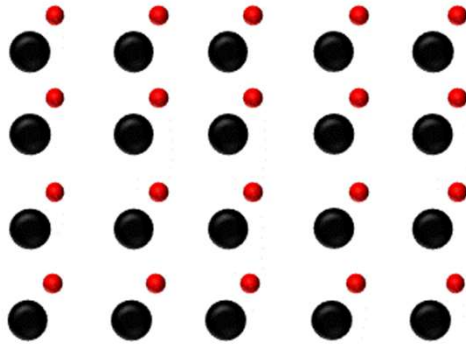
one atom, or a group of atoms

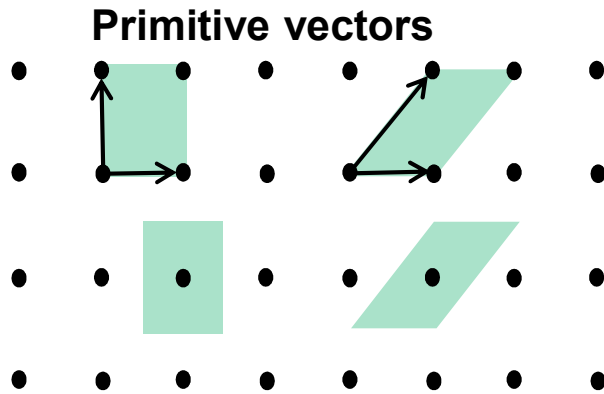- Every crystal has a corresponding Bravais lattice and a basis.

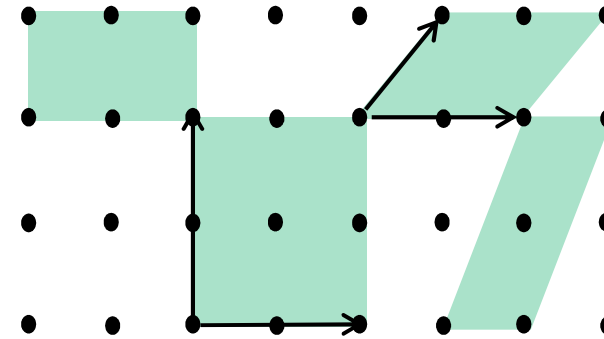 Note: *Lattice* is a math term, while *crystal* is a physics term.

  晶格   晶體

scienceline.ucsb.edu/getkey.php?key=4630

Unit cell (晶胞)

primitive cell (原始晶胞)   non-primitive cell

Primitive vectors

- A primitive cell contains only 1 lattice point (the choices are infinite).

- A non-primitive cell contains 2 or more lattice points.

  – For *Bravais* lattice, a unit cell can be primitive *or* non-primitive

  – For *non-Bravais* lattice, a unit cell is *always* non-primitive

- The sizes of a unit cell $(a_1. a_2, a_3)$ are called lattice constants

晶格常數

A special primitive cell: Wigner-Seitz (WS) cell

• Method of construction (works in 1D, 2D, 3D)
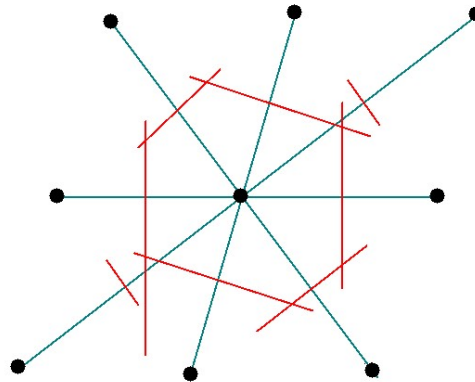
• The WS cell enclosing a lattice point is the region of space

that is closer to that lattice point than to any others.

• Advantage of the WS cell:

It has the same symmetry as the lattice

(symmetry here means translation, inversion, and rotation)
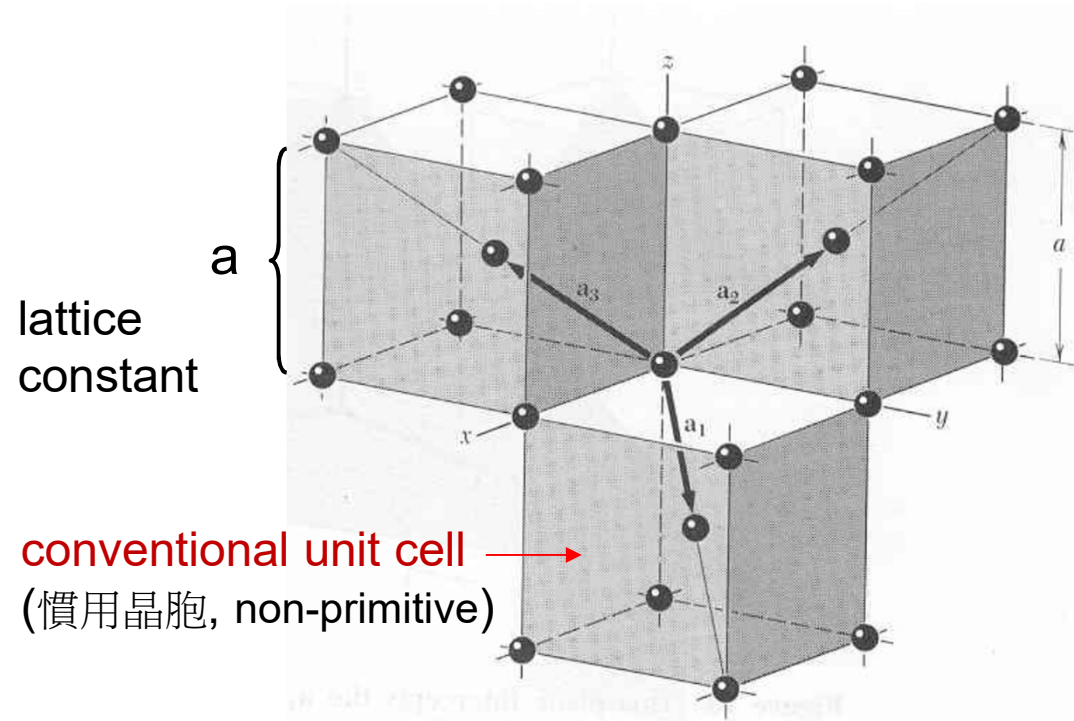
Crystal structures of *elements*

ccp (cubic close packing) = fcc

Note: It's rare to see simple cubic lattice.

chemicalstructure.net/portfolio/magnesium-and-aluminum/

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

a

lattice
constant

conventional unit cell →
(慣用晶胞, non-primitive)
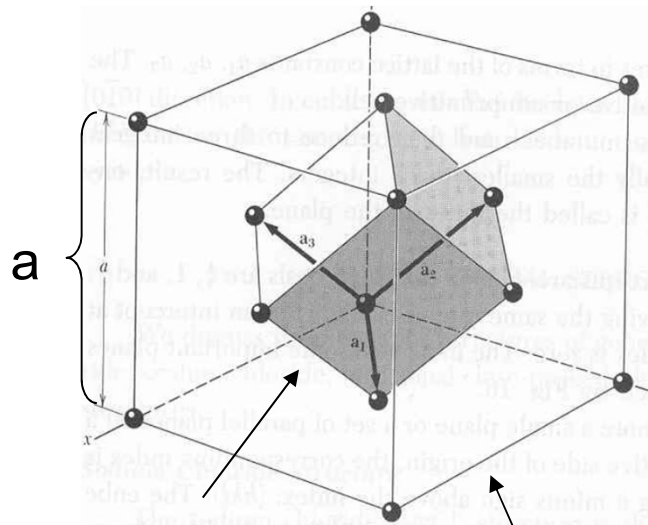
One possible choice
of *primitive* vectors

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

$$\vec{a}_2 = \frac{a}{2}(-\hat{x} + \hat{y} + \hat{z}),$$

$$\vec{a}_3 = \frac{a}{2}(\hat{x} - \hat{y} + \hat{z}).$$

• A bcc lattice is a Bravais lattice.

• For convenience of description, we can also treat it as

a simple cubic lattice with 2-point basis.

2). fcc lattice (Ne, Ar, Kr, Xe, Al, Cu, Ag, Au… etc)

a

A primitive unit cell

A conventional unit cell (non-primitive)

One possible choice of *primitive* vectors

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

$$\vec{a}_2 = \frac{a}{2}\left(\hat{y} + \hat{z}\right),$$

$$\vec{a}_3 = \frac{a}{2}\left(\hat{z} + \hat{x}\right).$$

Solid Ar at -189.3 C

- A fcc lattice is also a Bravais lattice.
- It can also be seen as a simple cubic lattice with 4-point basis.

3). hcp structure (Be, Mg… etc)

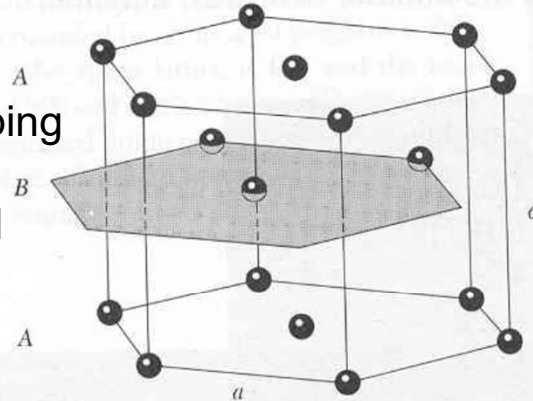2 overlapping "simple hexagonal lattices"

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 a_3 of Fig. 14.
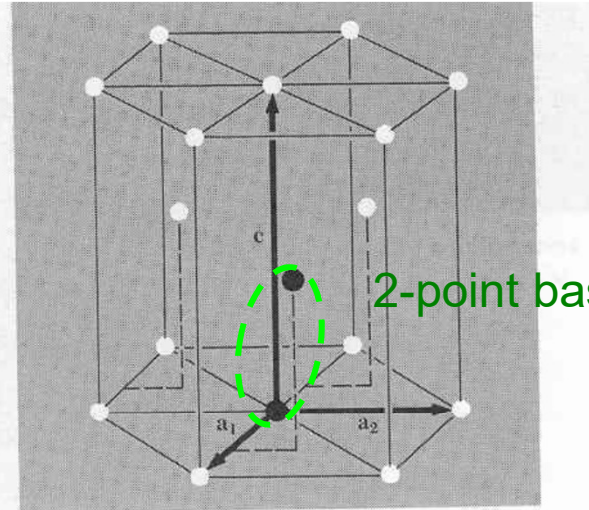
2-point basis

Figure 23 The primitive cell has $a_1 = a_2$, with an included angle of 120°. The c axis (or a_3) is normal to the plane of a_1 and 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 $\mathbf{r} = \frac{2}{3}\mathbf{a_1} + \frac{1}{3}\mathbf{a_2} + \frac{1}{2}\mathbf{a_3}$.
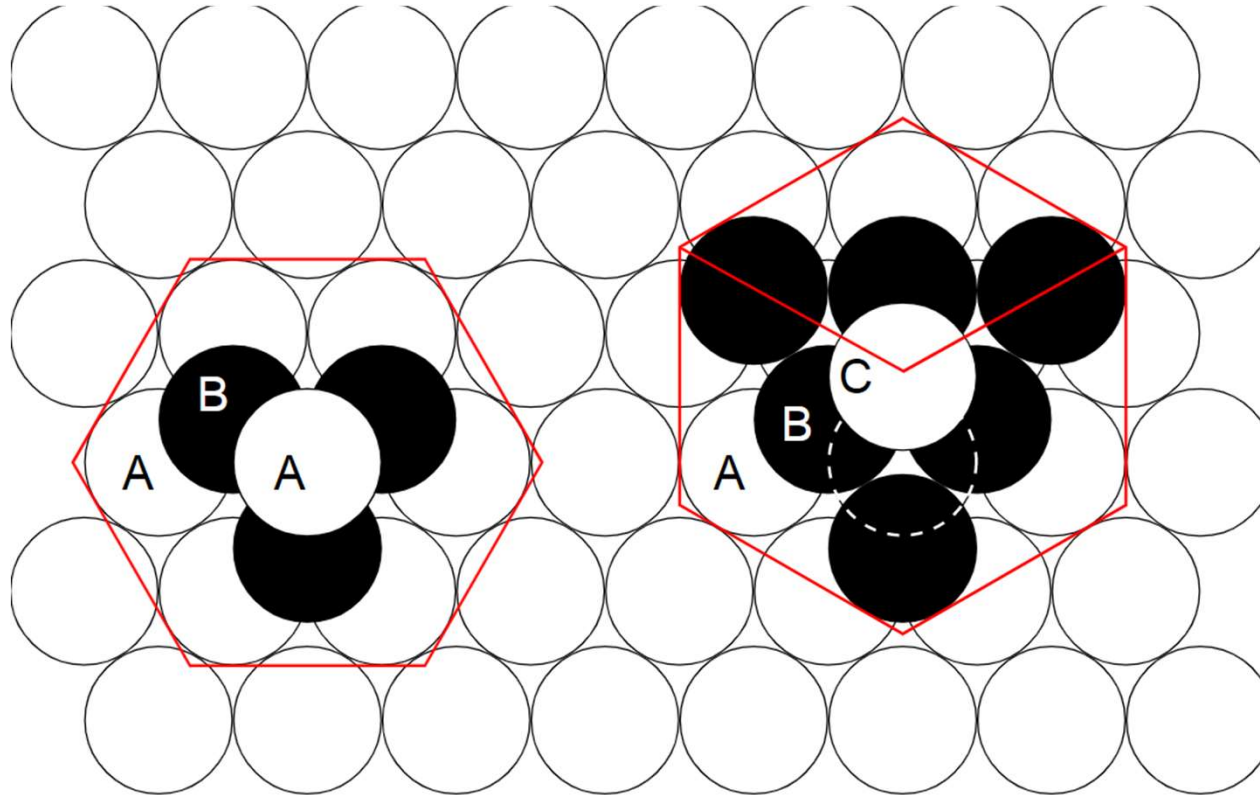
- hcp structure = simple hexagonal lattice + 2-point basis
- Primitive vectors: $\mathbf{a_1}$, $\mathbf{a_2}$, $\mathbf{c}$ [$\mathbf{c}$=2$\mathbf{a}$√ (2/3) for hcp, see Prob.5]
- The 2 atoms of the basis are located at
  $\mathbf{d_1}$=0, $\mathbf{d_2}$ = (2/3) $\mathbf{a_1}$+ (1/3) $\mathbf{a_2}$+(1/2)$\mathbf{c}$

The tightest way to pack spheres in 3D:
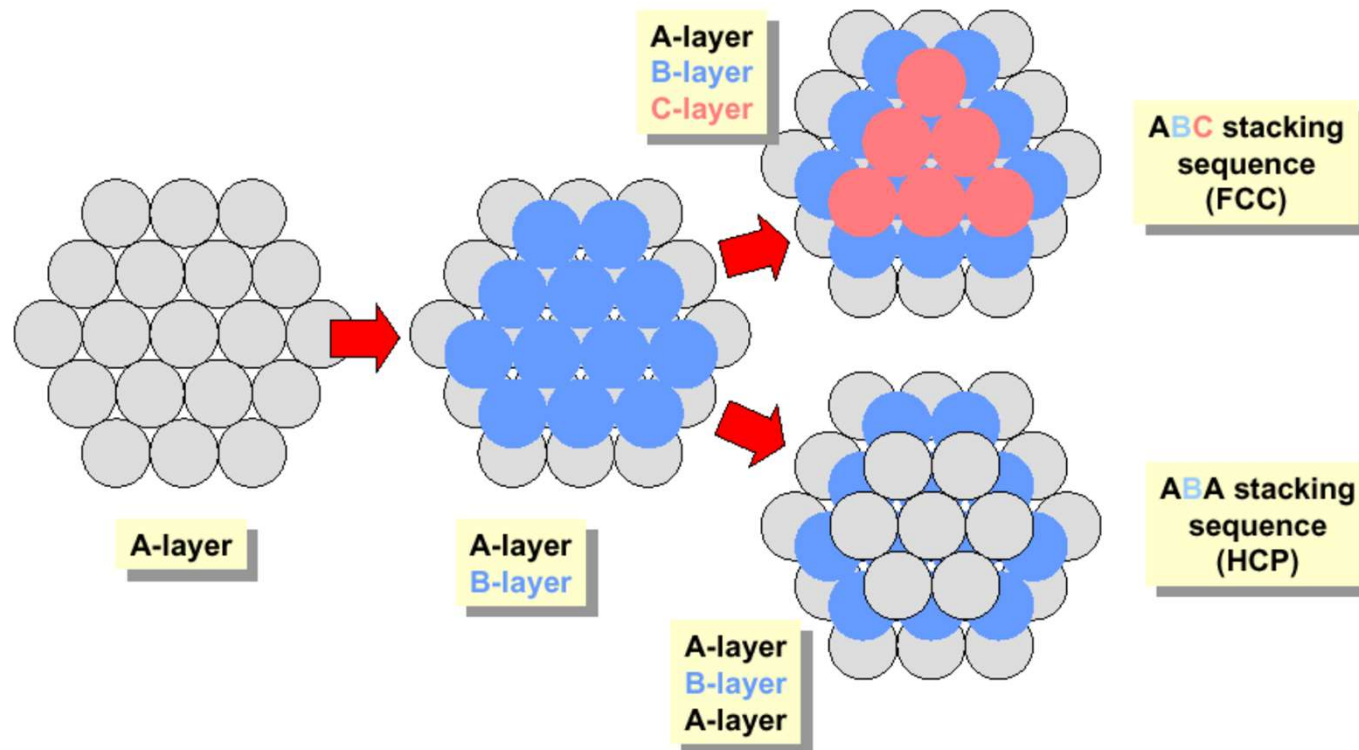
- ABCABC …= fcc

- ABAB …= hcp

- Other close packed structures: ABABCAB… etc.

Viewing from different angles

- Coordination number (配位數) = 12, packing fraction $\sim$ 74%   see Prob.6

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

Wiki: close packing of equal spheres

Kepler's conjecture (1611): The packing fraction of spheres in 3-dim ≦ π/√18

(the value of fcc and hcp)

Does the proof stack up?

Think peer review takes too long? One mathematician has waited four years to have his paper refereed, only to hear that the exhausted reviewers can't be certain whether his proof is correct. George Szpiro investigates.
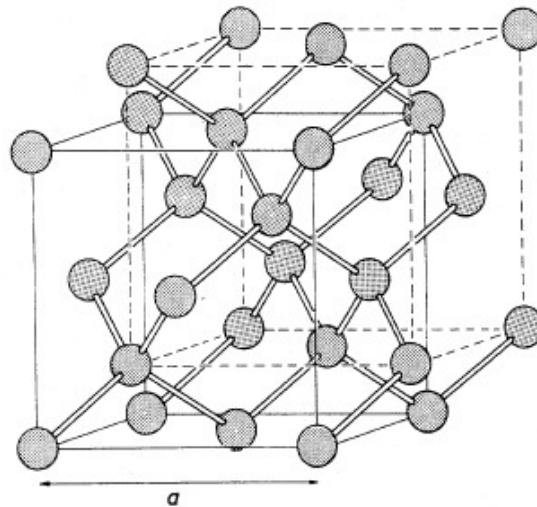

Grocers the world over know the most efficient way to stack spheres — but a mathematical proof for the method has brought reviewers to their knees.

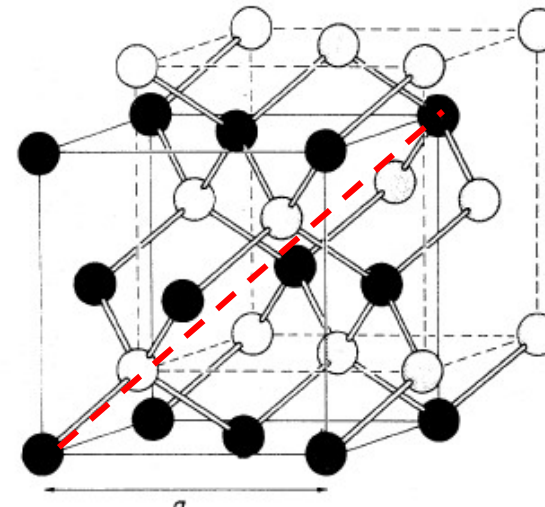(By the way, *nobody* can show that the crystalline form has the lowest energy.)

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

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

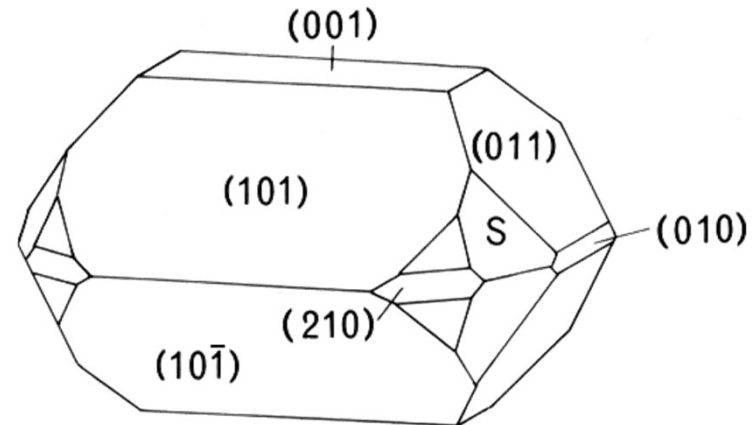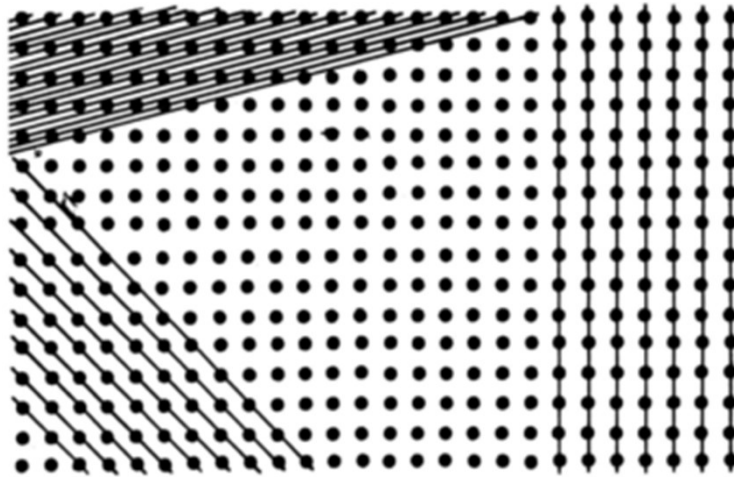= fcc lattice + 2-point basis, $d_1=0$, $d_2=(a/4)(x+y+z)$

diamond-type (Si, Ge)   ZnS-type (GaAs)

• Very low packing fraction ($\sim$36%!)   see Prob.6

• If the two atoms on the basis are different, then it is called
Zincblend (閃鋅) structure (eg. GaAs, ZnS… etc), which is a
familiar structure with an unfamiliar name.

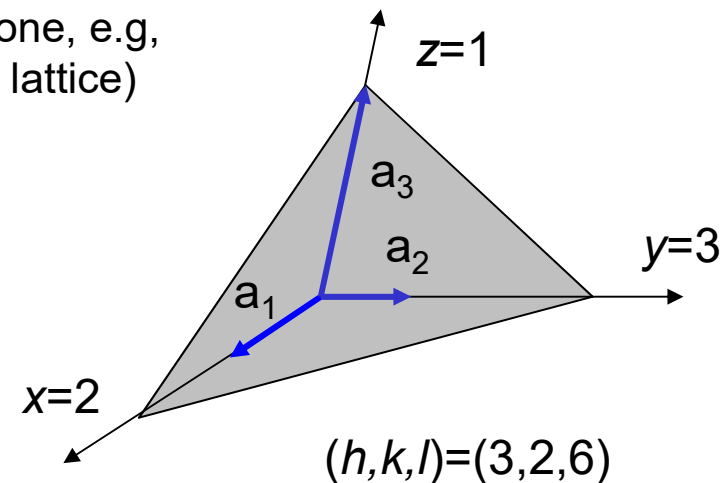# Indexing crystal planes: Miller index (h,k,l)

An Indexed PbSO$_4$ Crystal
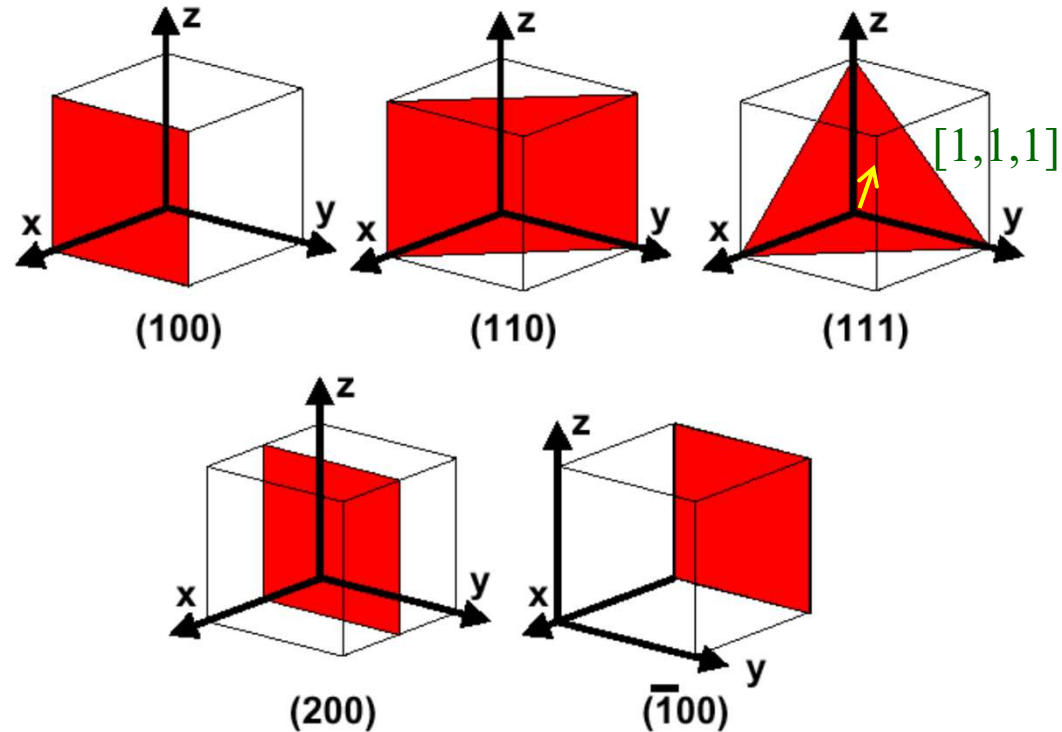
primitive vectors of Bravais lattice
(but not always the simplest one, e.g, the simple cubic lattice of fcc lattice)

The rules:

1. 取截距 (以$\mathbf{a_1}$, $\mathbf{a_2}$, $\mathbf{a_3}$為單位)
得 (x, y, z)

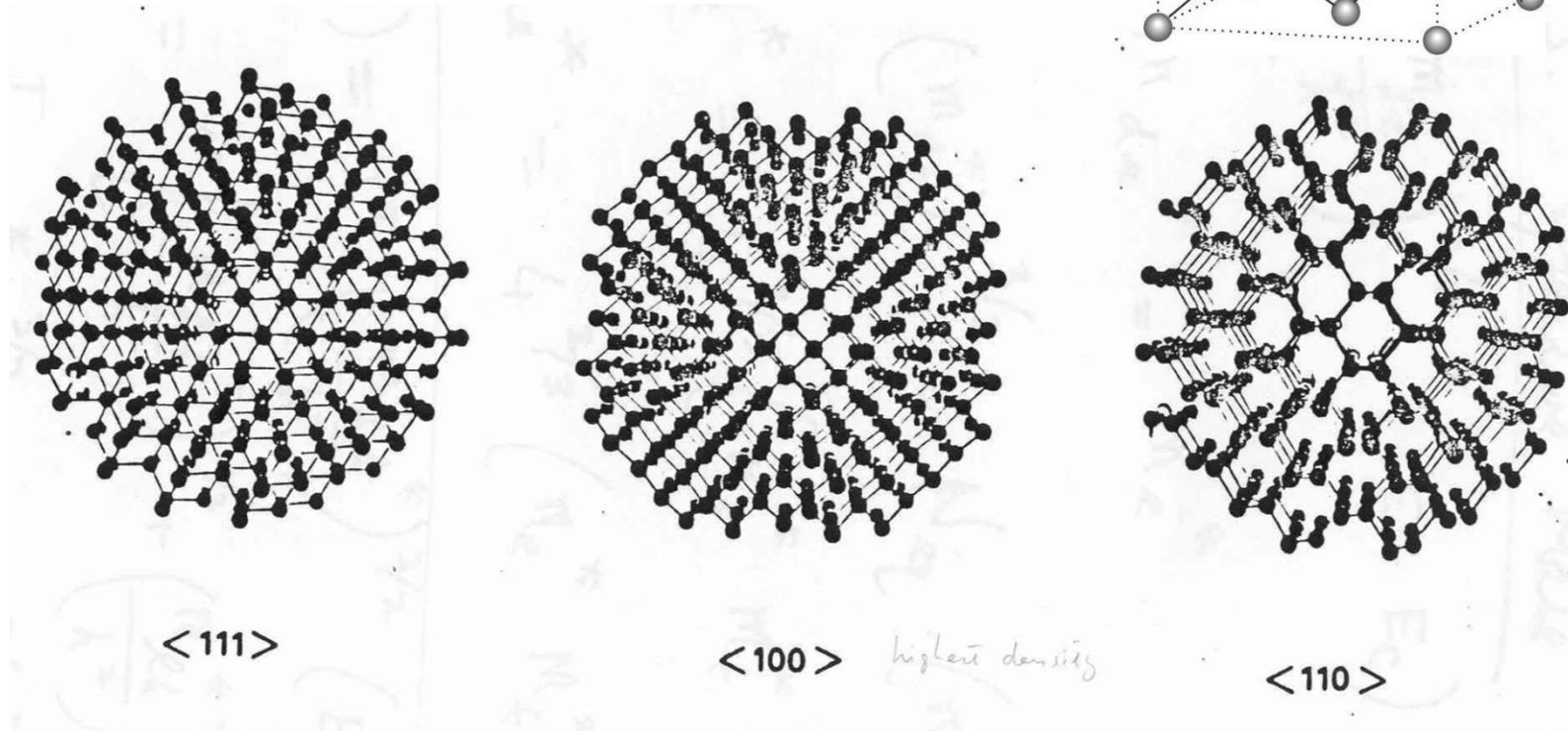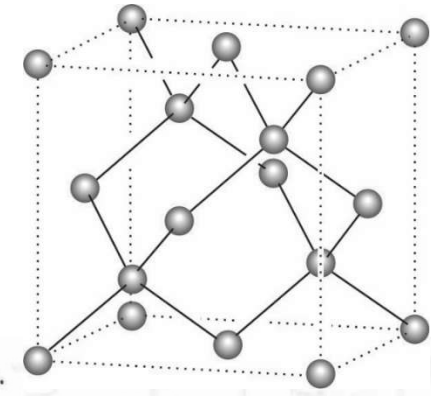2. 取倒數 ($1/x, 1/y, 1/z$)

3. 通分成互質整數 (h,k,l)

(h,k,l)=(3,2,6)

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

(100)   (110)   (111) [1,1,1]

(200)   ($\bar{1}$00)

• Square bracket [h,k,l] refers to the "direction" $h\mathbf{a}_1 + k\mathbf{a}_2 + l\mathbf{a}_3$, instead of crystal planes!

• For cubic crystals, [h,k,l] direction $\perp$ (h,k,l) planes

Diamond structure (eg. C, Si or Ge)

Termination of 3 low-index surfaces:

<111>   <100> highest density   <110>

- $\{h,k,l\}$ = (h,k,l)-plane + those equivalent to it by crystal symmetry
- $<h,k,l>$= $[h,k,l]$-direction + those equivalent to it by crystal symmetry