

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

<u>Material</u>	<u>Structure</u>	<u>Shape</u>	<u>Properties</u>
metal semiconductor insulator <i>superconductor</i> <i>magnetic</i> ... etc	crystal amorphous 非晶質 quasicrystal 準晶 ... etc	bulk surface interface nanocluster ... etc	mechanical thermal electrical magnetic optical ... etc

$$\text{Solid state physics} = \{A\} \times \{B\} \times \{C\} \times \{D\} \times \dots$$

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

Chap 1 Crystal structure

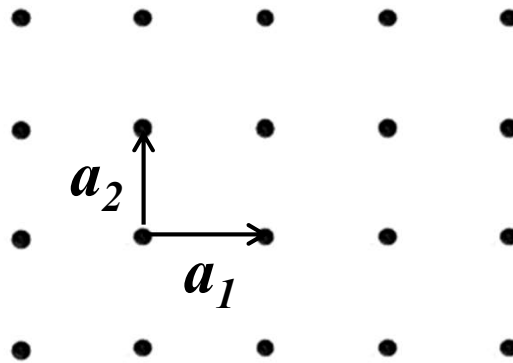


Dept of Phys



M.C. Chang

- A **primitive lattice** (in 3D) = a set of points with positions at $\mathbf{r} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$ (n_1, n_2, n_3 cover *all* integers), $\mathbf{a}_1, \mathbf{a}_2$, and \mathbf{a}_3 are called **primitive (translation) vectors** 原始向量



Alternative definition:

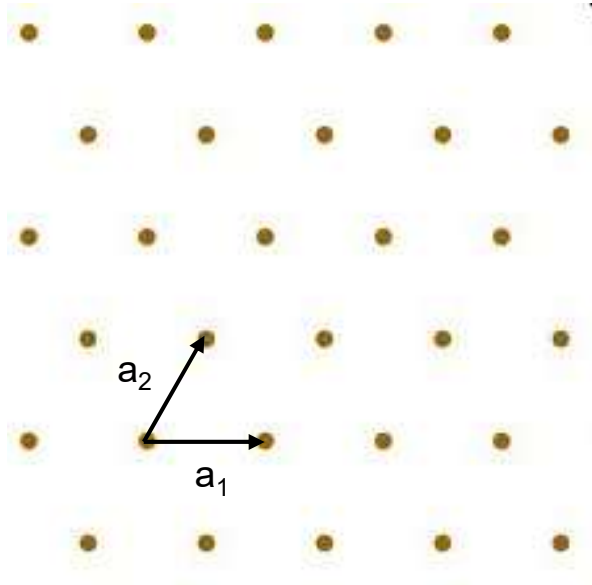
- A **primitive lattice** = a set of points in which every point has exactly the same environment.

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

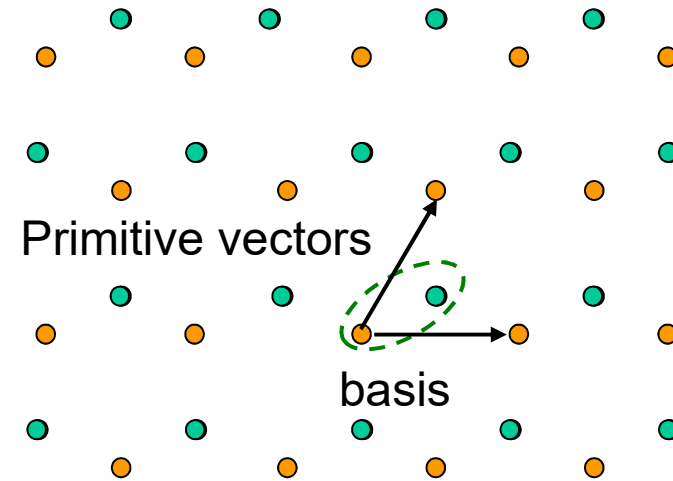
For example,
Triangular (or hexagonal) lattice



non-Bravais lattice

= Bravais lattice + **basis** 基元

Honeycomb lattice

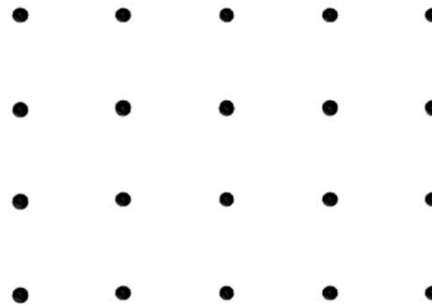
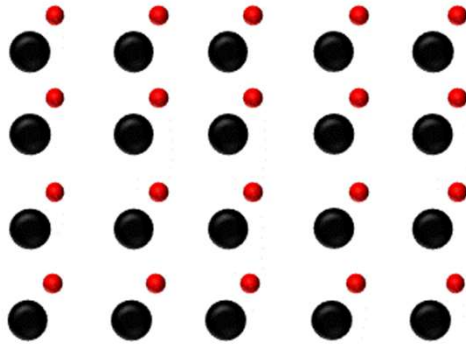


Honeycomb lattice =
triangular lattice + 2-point basis
(i.e. overlap of 2 triangular lattices)

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.

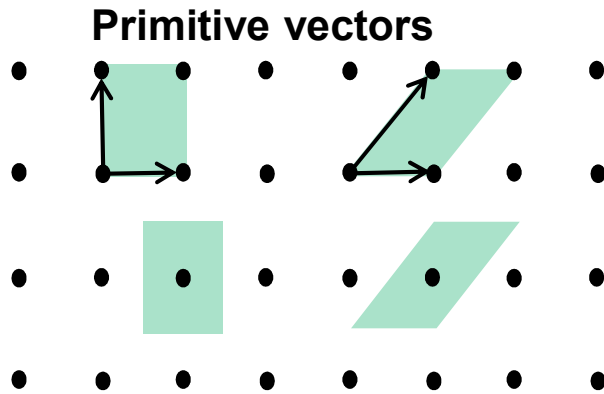
Note: *Lattice* is a math term, while *crystal* is a physics term.

晶格

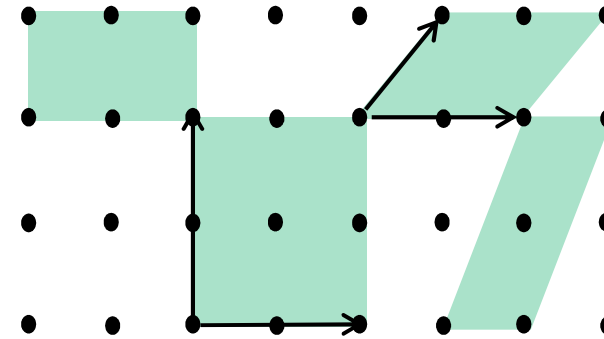
晶體

Unit cell (晶胞)

primitive cell (原始晶胞)



non-primitive cell

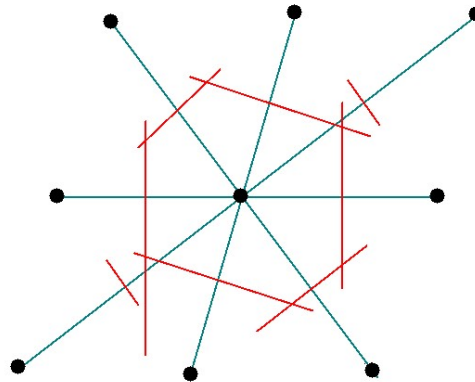


- A **primitive cell** contains only 1 lattice point (the choices are infinite).
- A **non-primitive cell** contains 2 or more lattice points.
 - For *Bravais* lattice, a unit cell can be primitive **or non-primitive**
 - For *non-Bravais* lattice, a unit cell is *always* non-primitive
- The sizes of 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*

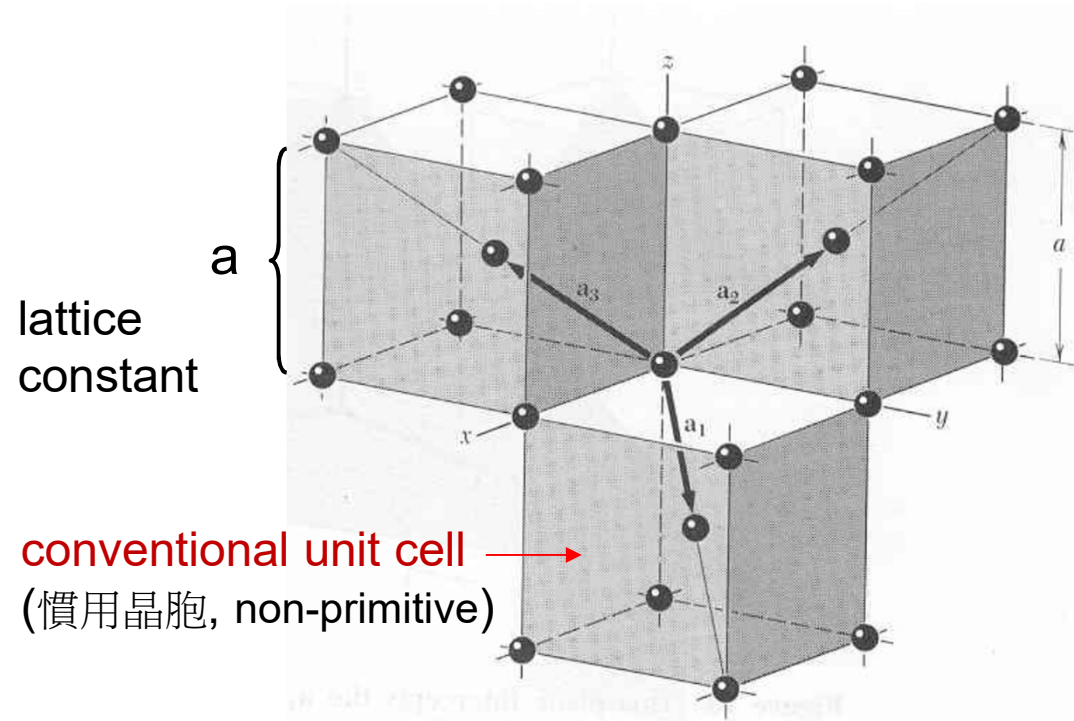
1 H Hydrogen other																	2 He Helium hcp				
3 Li Lithium bcc	4 Be Beryllium hcp															5 B Boron other	6 C Carbon other	7 N Nitrogen other	8 O Oxygen other	9 F Fluorine other	10 Ne Neon ccp
11 Na Sodium bcc	12 Mg Magnesium hcp															13 Al Aluminum ccp	14 Si Silicon other	15 P Phosphorus other	16 S Sulfur other	17 Cl Chlorine other	18 Ar Argon ccp
19 K Potassium bcc	20 Ca Calcium ccp	21 Sc Scandium hcp	22 Ti Titanium hcp	23 V Vanadium bcc	24 Cr Chromium bcc	25 Mn Manganese bcc	26 Fe Iron bcc	27 Co Cobalt hcp	28 Ni Nickel ccp	29 Cu Copper ccp	30 Zn Zinc hcp	31 Ga Gallium other	32 Ge Germanium other	33 As Arsenic other	34 Se Selenium other	35 Br Bromine other	36 Kr Krypton ccp				
37 Rb Rubidium bcc	38 Sr Strontium other	39 Y Yttrium hcp	40 Zr Zirconium hcp	41 Nb Niobium bcc	42 Mo Molybdenum bcc	43 Tc Technetium hcp	44 Ru Ruthenium hcp	45 Rh Rhodium ccp	46 Pd Palladium ccp	47 Ag Silver ccp	48 Cd Cadmium hcp	49 In Indium other	50 Sn Tin other	51 Sb Antimony other	52 Te Tellurium other	53 I Iodine other	54 Xe Xenon ccp				
55 Cs Cesium bcc	56 Ba Barium bcc	57 La Lanthanum dhcp	72 Hf Hafnium hcp	73 Ta Tantalum bcc	74 W Tungsten bcc	75 Re Rhenium hcp	76 Os Osmium hcp	77 Ir Iridium ccp	78 Pt Platinum ccp	79 Au Gold ccp	80 Hg Mercury other	81 Tl Thallium hcp	82 Pb Lead ccp	83 Bi Bismuth other	84 Po Polonium pc	85 At Astatine ccp	86 Rn Radon ccp				
87 Fr Francium bcc	88 Ra Radium bcc	89 Ac Actinium ccp	104 Rf Rutherfordium other	105 Db Dubnium other	106 Sg Seaborgium other	107 Bh Bohrium other	108 Hs Hassium other	109 Mt Meitnerium other	110 Ds Darmstadtium other	111 Rg Roentgenium other	112 Cn Copernicium other	113 Uut Ununtrium other	114 Fl Flerovium other	115 Uup Ununpentium other	116 Lv Livermorium other	117 Uus Ununseptium other	118 Uuo Ununoctium other				

ccp (cubic close packing) = fcc

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

58 Ce Cerium dhcp	59 Pr Praseodymium dhcp	60 Nd Neodymium dhcp	61 Pm Promethium dhcp	62 Sm Samarium other	63 Eu Europium bcc	64 Gd Gadolinium hcp	65 Tb Terbium hcp	66 Dy Dysprosium hcp	67 Ho Holmium hcp	68 Er Erbium hcp	69 Tm Thulium hcp	70 Yb Ytterbium ccp	71 Lu Lutetium hcp
90 Th Thorium ccp	91 Pa Protactinium other	92 U Uranium other	93 Np Neptunium other	94 Pu Plutonium other	95 Am Americium dhcp	96 Cm Curium dhcp	97 Bk Berkelium dhcp	98 Cf Californium dhcp	99 Es Einsteinium ccp	100 Fm Fermium other	101 Md Mendelevium other	102 No Nobelium other	103 Lr Lawrencium other

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



One possible choice of *primitive* vectors

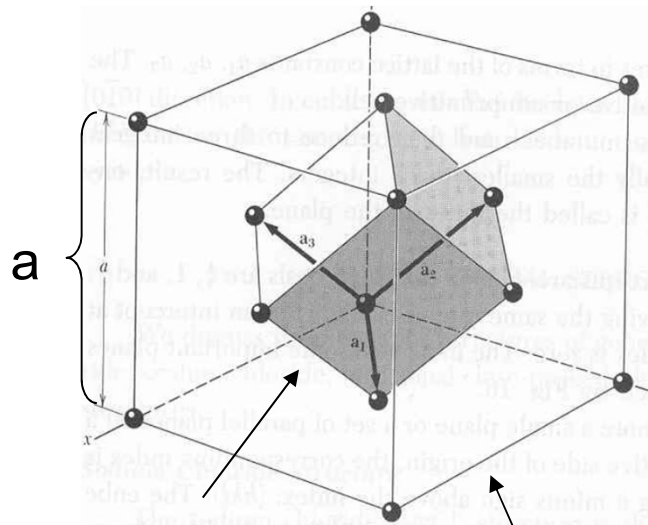
$$\vec{a}_1 = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z}),$$

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

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

- 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 primitive
unit cell

A conventional
unit cell (non-
primitive)

One possible choice
of *primitive* vectors

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

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

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



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”

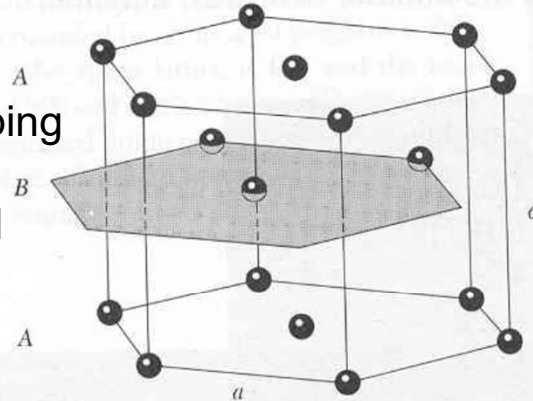


Figure 22 The hexagonal close-packed structure. The atom positions in this structure do not constitute a space lattice. The space lattice is simple hexagonal with a basis of two identical atoms associated with each lattice point. The lattice parameters a and c are indicated, where a is in the basal plane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

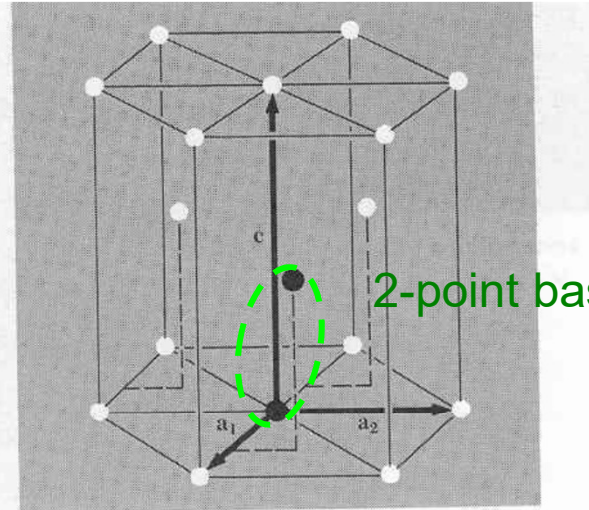
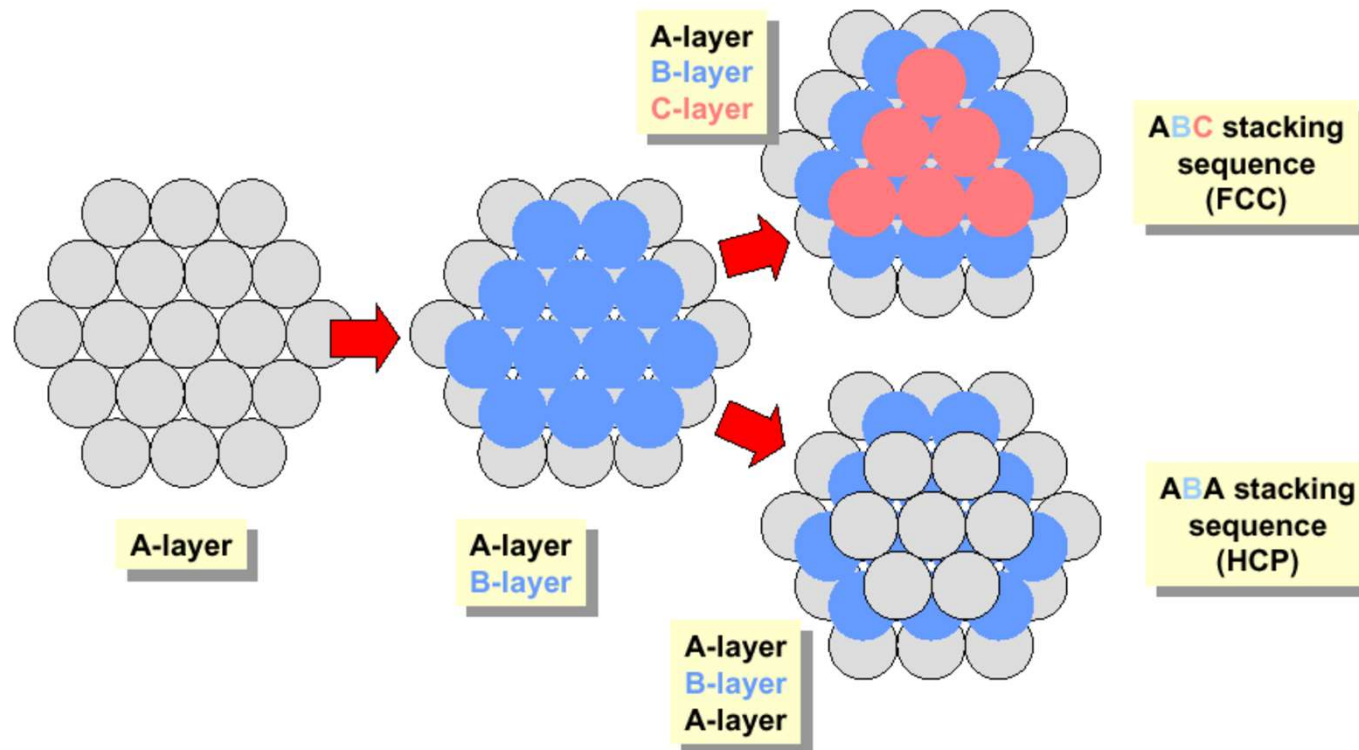


Figure 23 The primitive cell has $a_1 = a_2$, with an included angle of 120° . The c axis (or \mathbf{a}_3) is normal to the plane of \mathbf{a}_1 and \mathbf{a}_2 . The ideal hcp structure has $c = 1.633 a$. The two atoms of one basis are shown as solid circles. One atom of the basis is at the origin;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

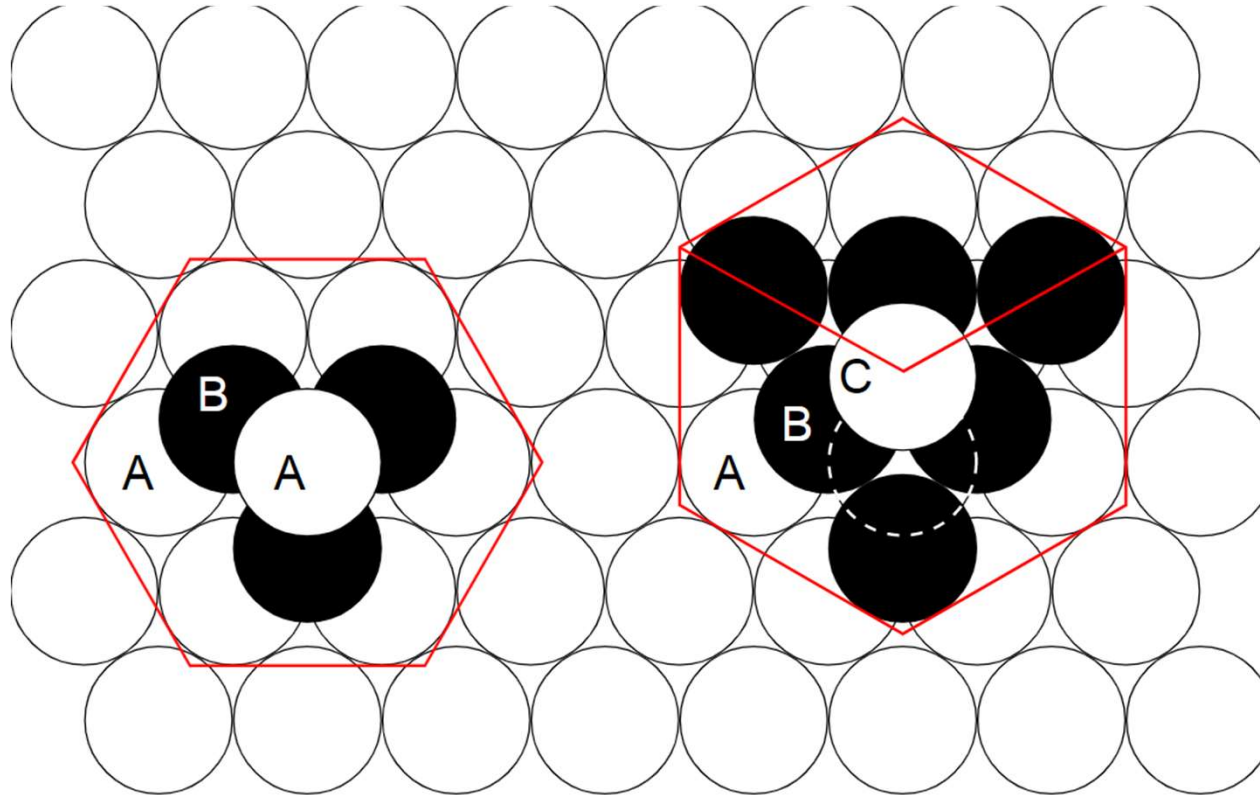
- hcp structure = simple hexagonal lattice + 2-point basis
- Primitive vectors: $\mathbf{a}_1, \mathbf{a}_2, \mathbf{c}$ [$\mathbf{c} = 2a\sqrt{2/3}$ for hcp, see Prob.5]
- The 2 atoms of the basis are located at
 $\mathbf{d}_1 = 0, \mathbf{d}_2 = \frac{2}{3}\mathbf{a}_1 + \frac{1}{3}\mathbf{a}_2 + \frac{1}{2}\mathbf{c}$

The tightest way to pack spheres in 3D:



- ABCABC ...= fcc
- ABAB ...= hcp
- Other close packed structures: ABABCAB... etc.

Viewing from different angles



- **Coordination number (配位数) = 12**, packing fraction $\sim 74\%$ see Prob.6
(Cf: bcc, coordination number = 8, packing fraction $\sim 68\%$)

Kepler's conjecture (1611): The packing fraction of spheres in 3-dim $\leq \pi/\sqrt{18}$

Does the proof stack up?

(the value of fcc and hcp)

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.



Nature, 3 July 2003

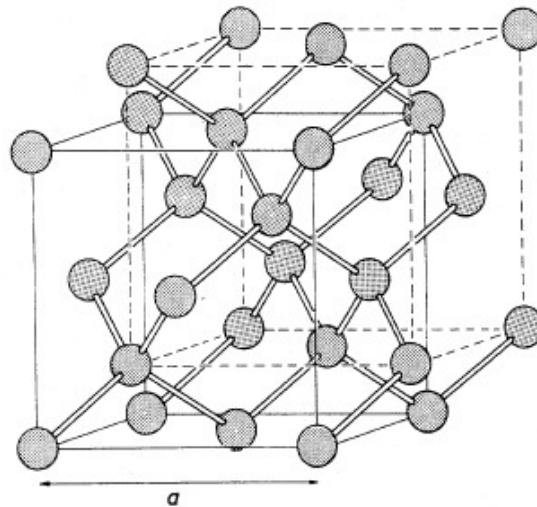
Grocers the world over know the most efficient way to stack spheres — but a mathematical proof for the method has brought reviewers to their knees.

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

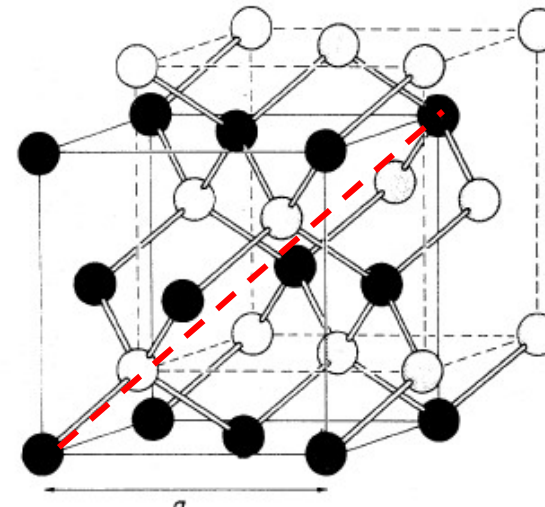
4). Diamond structure (C, Si, Ge... etc)

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

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



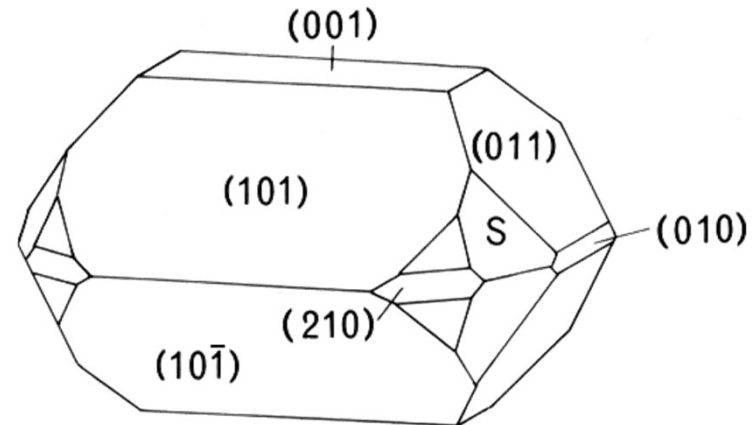
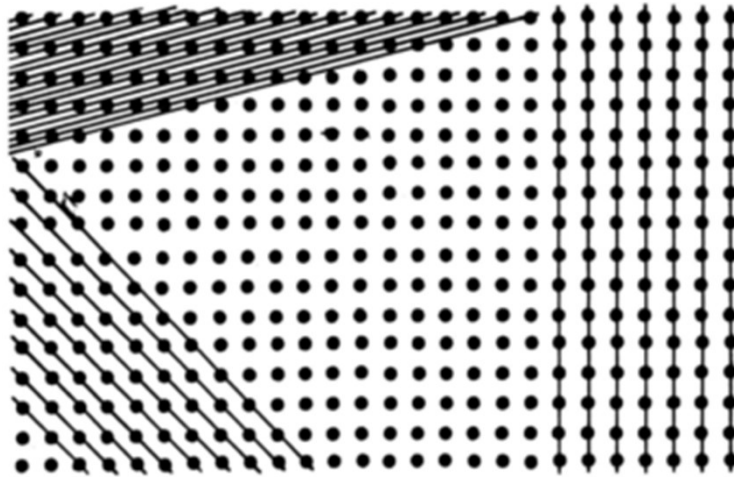
diamond-type (Si, Ge)



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 **Zincblende (閃鋅) structure** (eg. GaAs, ZnS... etc), which is a familiar structure with an unfamiliar name.

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



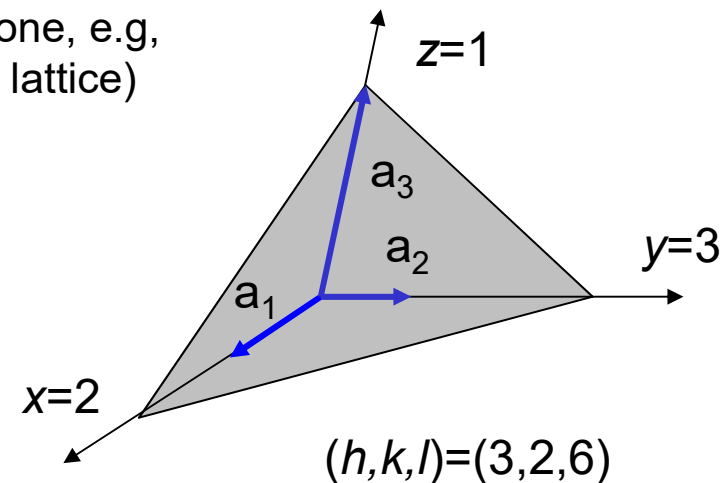
An Indexed PbSO_4 Crystal

primitive vectors of Bravais lattice

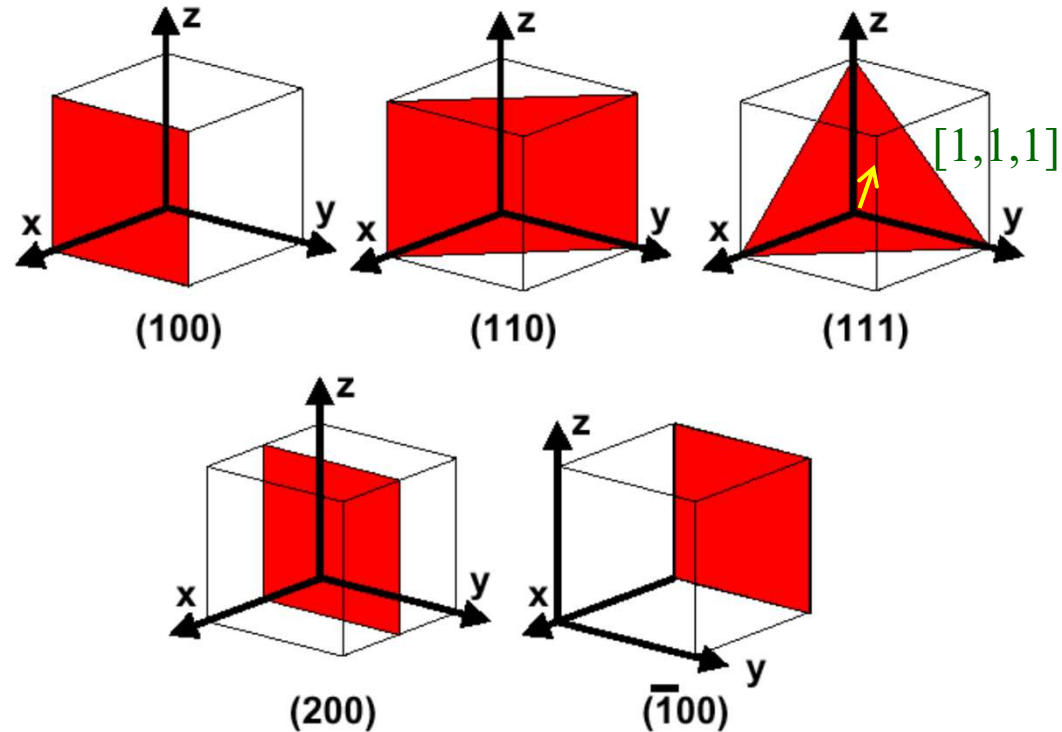
(but not always the simplest one, e.g, the simple cubic lattice of fcc lattice)

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)



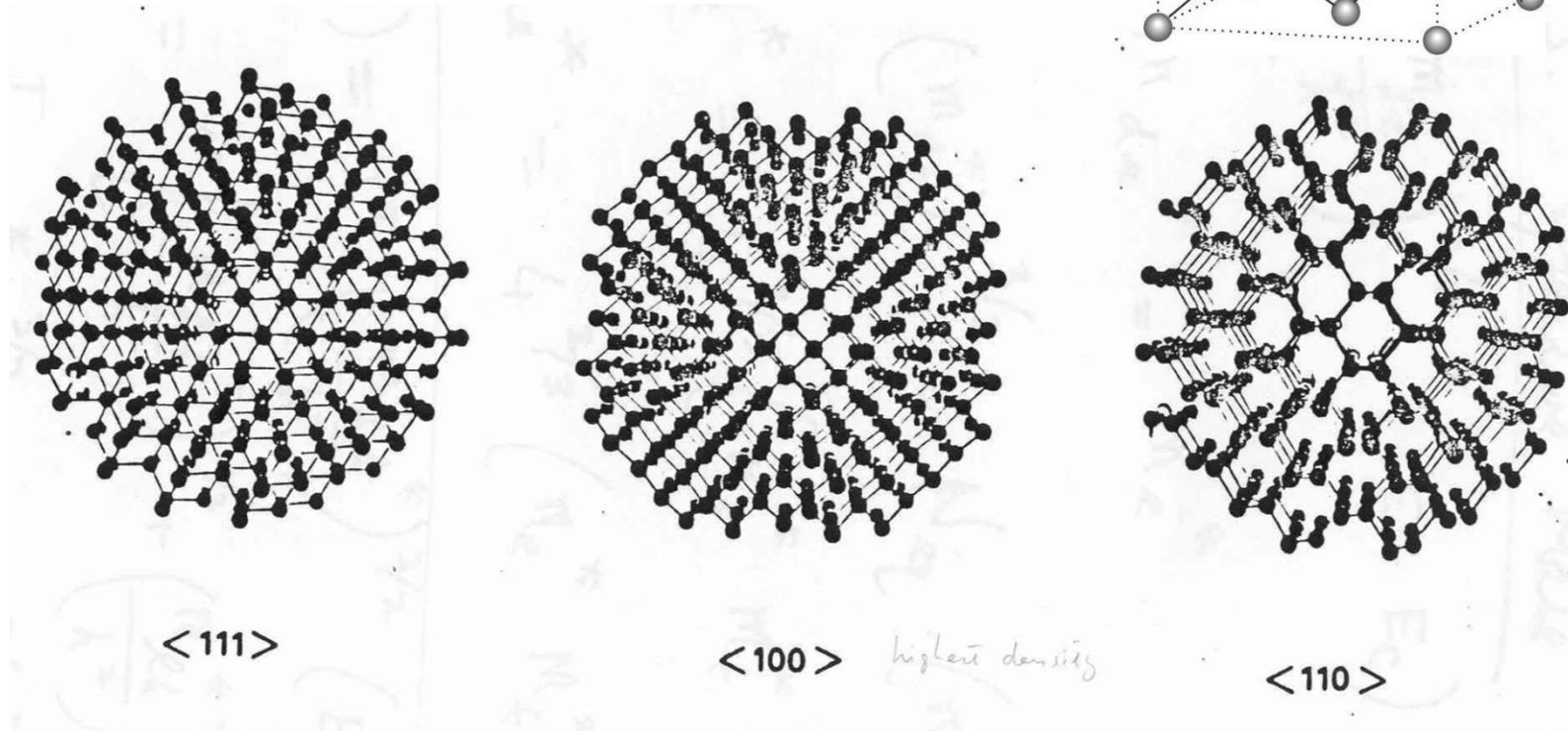
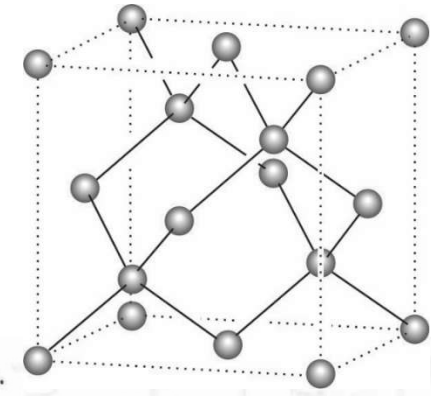
For example, cubic crystals (including bcc, fcc... etc)



- Square bracket $[h,k,l]$ refers to the “direction” $ha_1+ka_2+la_3$, 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:



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