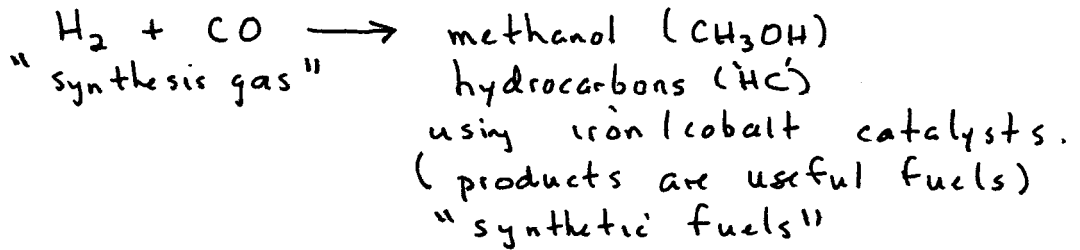


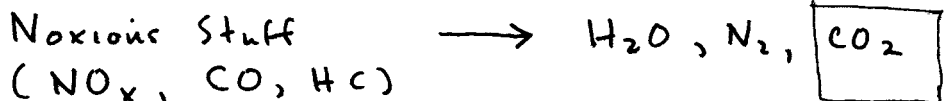
2. Fischer - Tropsch Chemistry

coal
biomass



3. "Threeway" Catalyst

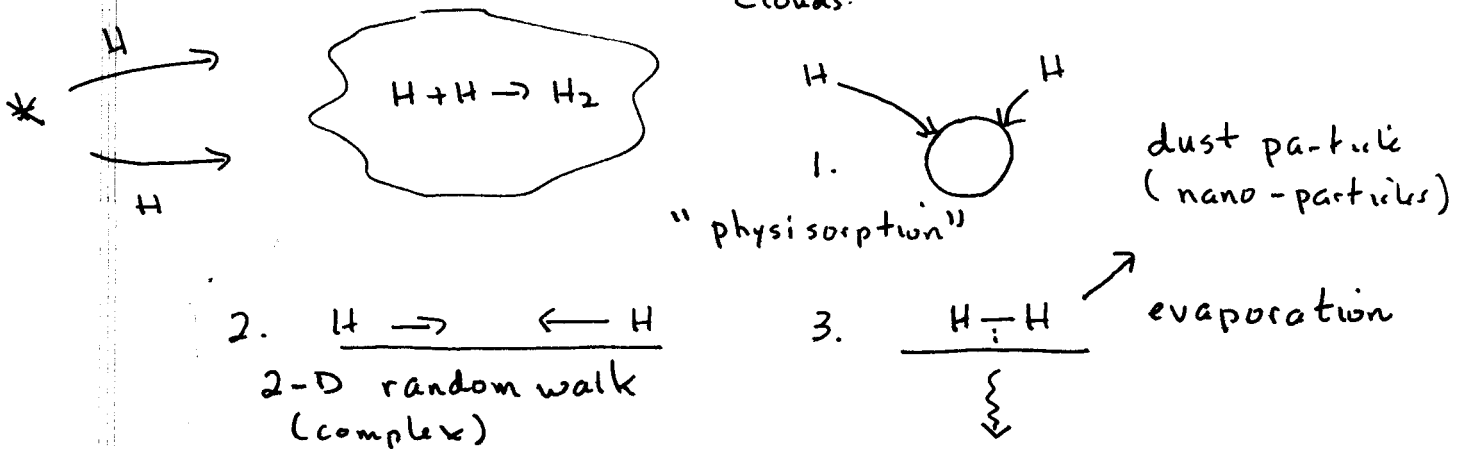
- automobile catalytic converter (Pt, Rh, Pd)



OK, but greenhouse problem
poisoned by Pb

In addition to active catalysts, surfaces can act as passive catalysts for reactions by just being there.

Most important example: conversion of atomic to molecular hydrogen in interstellar clouds.



On silicates (analogs of grains), process works between 10-20K.
 $T < 10 K$ no motion $T > 20 K$ evaporation of H.

Nanotechnology: Small devices can be crafted on surfaces, with ultra-high resolution down to the atomic level.

I. Bulk Solids + Crystallography

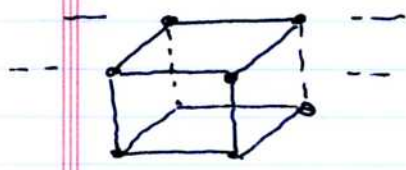
To understand surfaces, we should probably first review bulk solids; since by surfaces, we will be specifying gas - solid interfaces.

Crystalline: constituent atoms, molecules, ions, arranged in an orderly, repetitive pattern in three dimensions "long-range order"

Amorphous: perhaps some short-range order, but no long-range order. (e.g. amorphous carbon, amorphous ice)

Both can have irregular surfaces; crystal surfaces can have imperfections to perfect long-range order.

We will focus on crystalline solids, although interstellar grains are amorphous. Crystals can be divided into small units known as unit cells; e.g. a simple cubic cell:

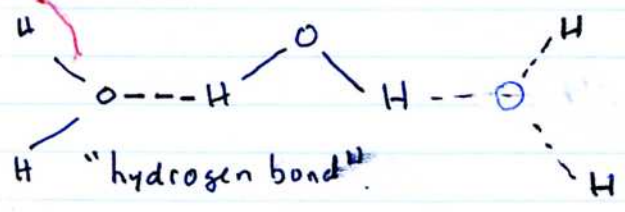


• basis can be atom or molecule. We will normally think in terms of atoms.

The structure of the unit cells depends upon the substance and the type of bonding, of which there are 4 main types:

- (i) metallic: cells composed of atoms (e.g. Fe) with delocalized electrons
- (ii) ionic: cells made up of pairs of ions (e.g. $\text{Na}^+ \text{Cl}^-$)
- (iii) van der Waals: cells made up of weakly bound molecules (ice) or atoms (Ar)

covalent



normally electrostatic except for hydrogen bonding

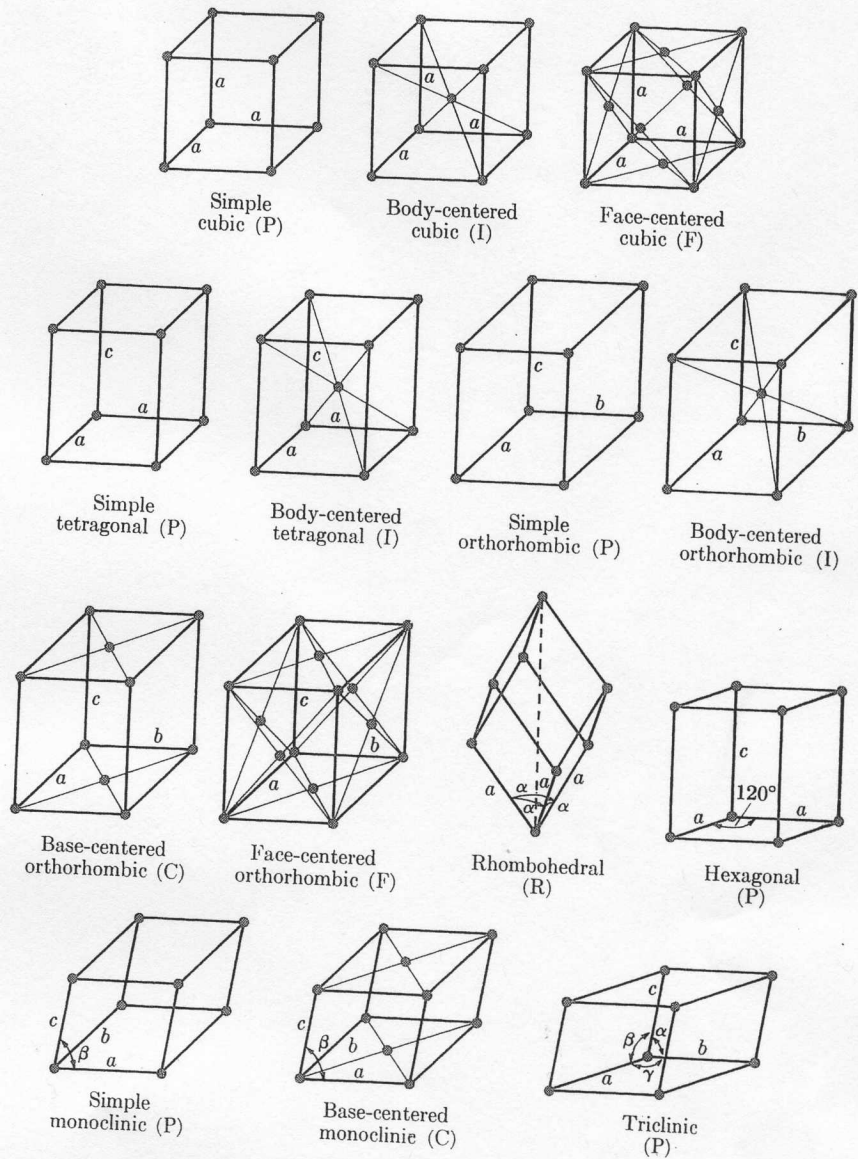


Fig. 26-20 The fourteen Bravais lattices.

In addition to the symmetry within any particular cell, the points in the neighboring cells are related by symmetry to those in that particular cell. Thus we can add symmetry operations which contain an element of translation as well as the other elements appropriate to the finite figure. The addition of translation to the possible

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(iv) covalent: strong, chemical bonds between atoms (diamond) hard to vaporize

Note: these can be mixed. An ionic or van der Waals crystal with a molecular basis has covalent bonds for the basis.

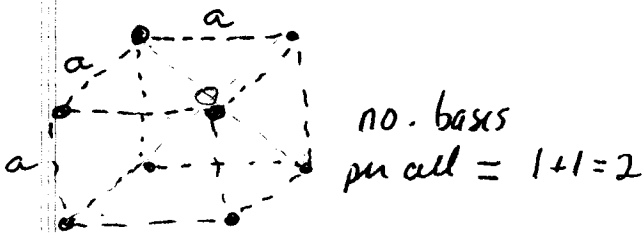
Bravais Lattices

We can think of unit cells as parts of a lattice with the points as bases.



In 1848, Bravais showed that all 3-D lattices can be divided into 14 types. (Castellan hand-out) Perhaps the three most important are:

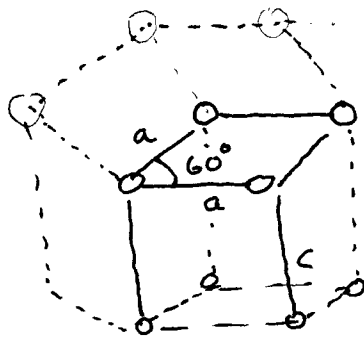
Body-Centered Cubic



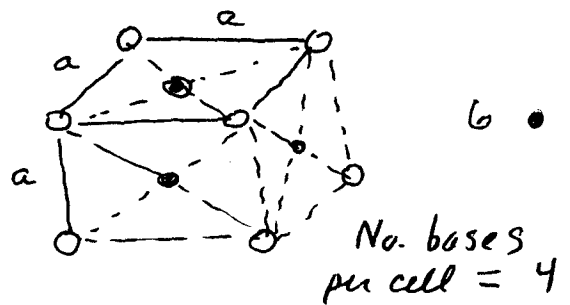
○ : along major diagonal $\sqrt{3}a$

Hexagonal

$c \neq a$

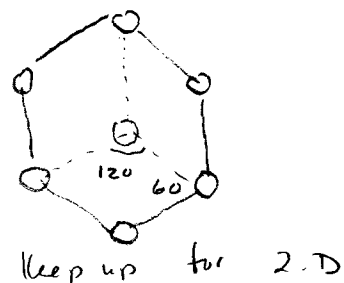


Face-Centered Cubic



(each face has a central basis) along face diagonal $\sqrt{2}a$

Top View

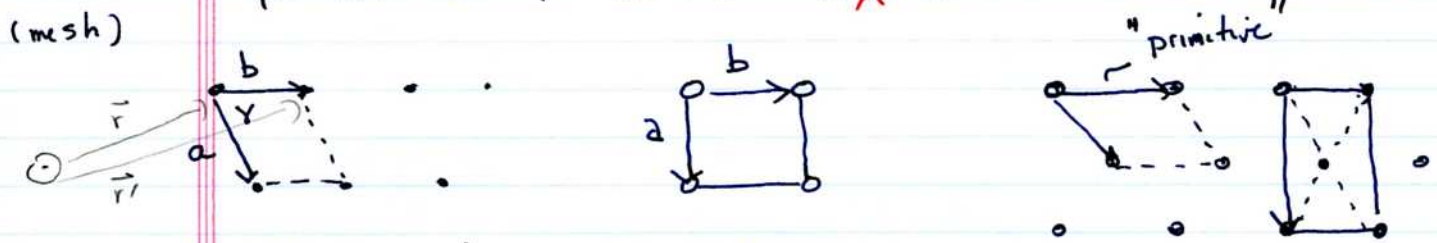


See web for actual lattice.

2-D Bravais Lattices

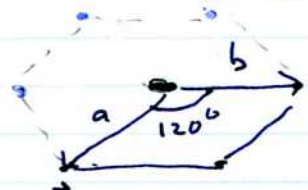
major?

In perfect 2-D, there are 5 Bravais Lattices:



1. Oblique
2. rectangular
3. (square)
4. centered rectangular

(note vector approach)



5. hexagonal ($|a| = |b|$)

$\vec{r}' = \vec{r} + n\vec{a} + m\vec{b}$ crystal looks same as viewed from $\vec{r} \cdot \vec{r}'$.

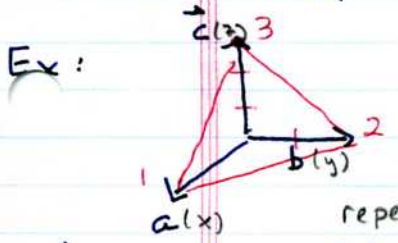
$n, m = 0, \pm 1, \pm 2$ etc.

Note: these lattices do not really represent surfaces of 3-D crystals well since the inner layers may also be important, as we shall see. Now proceed to more complex description of internal and external planes.

Ideal Crystal Faces & Miller Indices (hkl)

Miller Indices For Planes (Cut or given surface) or internal planes for X-ray diffraction.

1. Find the intercepts of the plane on the axes in terms of lattice constants a, b, c . Exclude origin.
2. Take the reciprocals of the obtained numbers.
3. Reduce to three integers having the same ratio, usually the smallest 3 integers.



Intercepts = 1, 2, 3 (x, y, z order)

Reciprocals = $1, \frac{1}{2}, \frac{1}{3}$

Smallest integers = 6, 3, 2 (6, 3, 2)

(+ all parallel planes)

'high index plane' (also works for intercepts 2, 4, 6)

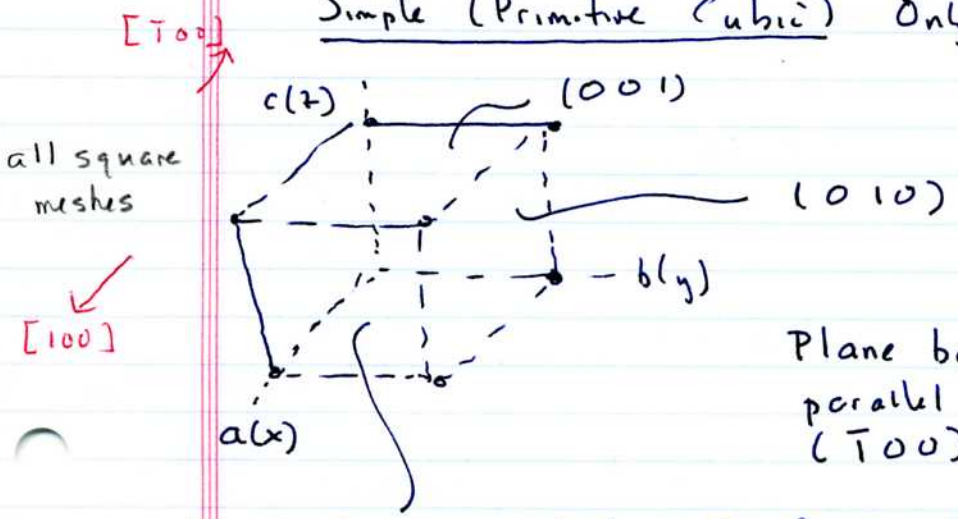
4. Also, if plane || to an axis, intercept is at ∞ and index is zero
5. If it is necessary to distinguish direction ($\vec{a} = 1\vec{a}$ vs $\vec{a} = -1\vec{a}$) can use a negative number. This convention is needed if one refers to a \perp vector rather than the plane. $[\] = \text{vector}$

Low Index Planes

Simple (Primitive Cubic)

Only in cubic crystals, the components $[hkl]$ are \perp to the plane (hkl)

Sometimes easier to find components in standard vector manner.

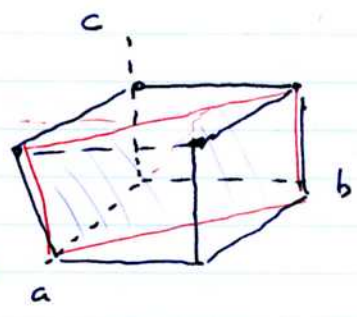


Plane behind origin with $\vec{r} = -\vec{a}$ parallel to 100 can be written $(\bar{1}00)$ $\bar{1} = -1$

$a, b, c = 1, \infty, \infty \rightarrow (100)$ front + back face etc.

(Use distance formula)

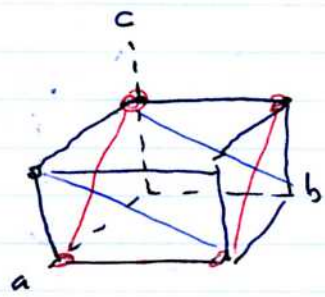
rectangular mesh



Intercepts

$a, b, c = 1, 1, \infty \Rightarrow (1, 1, 0)$

\perp vectors $[1, 1, 0]$ $[\bar{1} \bar{1} 0]$



Intercepts

$a, b, c = 1, \infty, 1 \Rightarrow (1, 0, 1)$

\perp vectors $[1 0 1]$ $[\bar{1} 0 \bar{1}]$

- Also

$a, b, c = \infty, 1, 1 \Rightarrow (0, 1, 1)$

\perp vectors $[0 1 1]$ $[0 \bar{1} \bar{1}]$

These are examples of "low index" planes, which are most commonly encountered. High index planes have layer & unequal intercepts & are encountered in lattices with non-primitive nature, where they are just not mainly empty space.