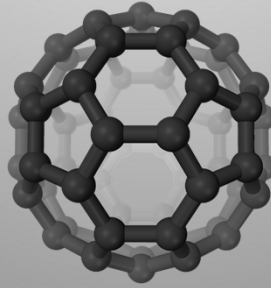
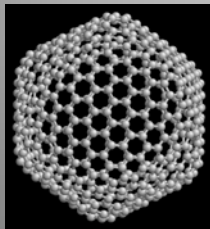
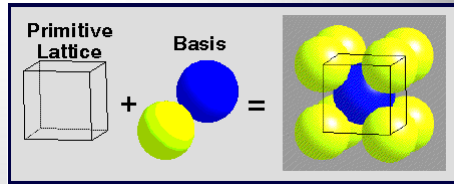


PHYS485 Materials Physics

Dr. Gregory W. Clark
Manchester University



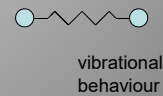
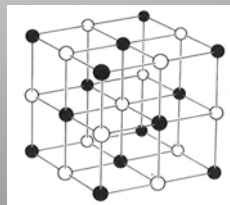
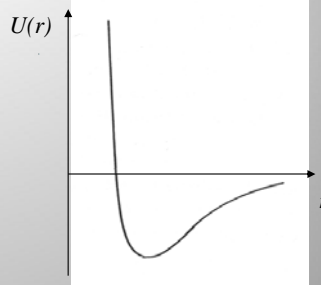
First generated in 1985 by Harold Kroto, James R. Heath, Sean O'Brien, Robert Curl, and Richard Smalley at Rice University. 1996 Nobel Prize in Chemistry

C₆₀ Buckminsterfullerene

tentative!

Outline for the First Half-Semester

- Bonding in Solids
- Static Structure of Crystals
- Dynamic Structure of Crystals
- Mechanical Properties
- Electrons in Solids



Periodic Table of the Elements

groups periods

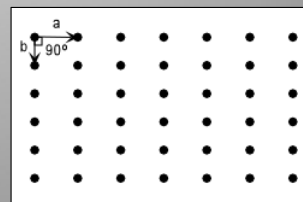
Direction of increasing +Z value

1s
2s 2p
3s 3p 3d
4s 4p 4d 4f
5s 5p 5d 5f ...
6s 6p 6d

Crystalline Solids



- Easiest to model/study:
 - **Translational invariance:** a crystal appears identical when viewed from all the positions given by a **lattice vector**
- The basics:
 - **Lattice:** group of geometric points defining atomic positions



Lattices

- Imagine space divided up by 3 sets of parallel equally-spaced planes:

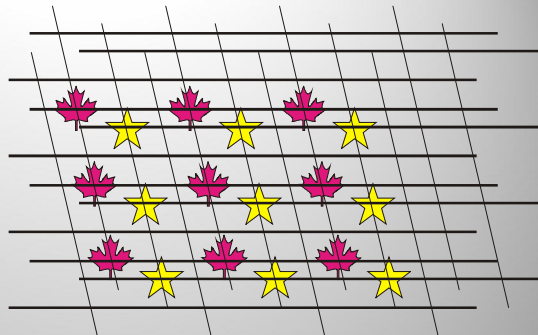


(in 2-dimensions [2D] here)

The points of intersection are referred to as **lattice points**.

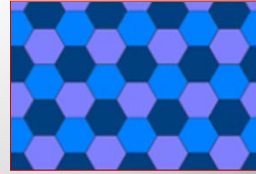
The lattice points constitute a regular array of points which are *indistinguishable*. Hence a lattice has no unique origin (**translational invariance**).

We can see that we can choose any origin for the lattice and the lattice points are always indistinguishable.



- The basics:
 - **Unit cell:** One of the identical cells defined by the intersecting planes is referred to as a **unit cell**. The **unit cell** is the building block of a crystal.
 - **Lattice parameter:** the distance between adjacent lattice points (in a given direction; three, in general)

Crystalline Solids



- Easiest to model/study:
 - **Translational invariance**: a crystal appears identical when viewed from all the positions given by a **lattice vector**
- The basics:
 - **Lattice**: group of geometric points defining atomic positions
 - **Lattice vectors**: a vector that takes us from one lattice point to any other lattice point
 - **Basis vectors (primitive axes)**: the smallest lattice vectors that span the space

Crystalline Solids

- Example:

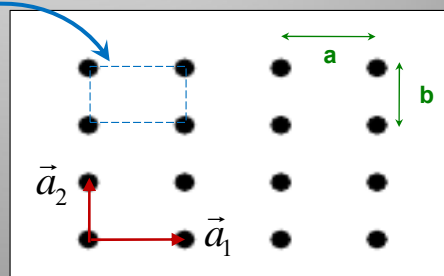
- 2D rectangular **lattice**:

- **Lattice vectors** $\left\{ \begin{array}{l} \vec{R} = n_1 a \hat{i} + n_2 b \hat{j} = n_1 \vec{a}_1 + n_2 \vec{a}_2 \\ \text{where the } \vec{a}_i \text{ are } \mathbf{basis\ vectors} \end{array} \right.$

choice is not unique, but only one is "conventional"

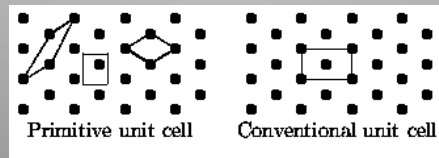
note we can draw a repeating **unit cell**

finally, note there is **one atom per unit cell**



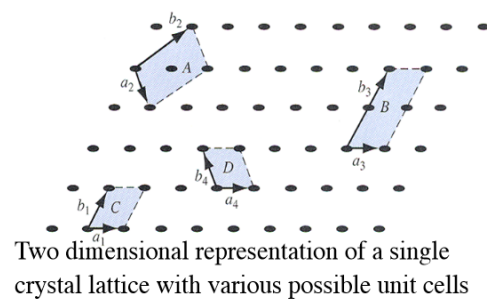
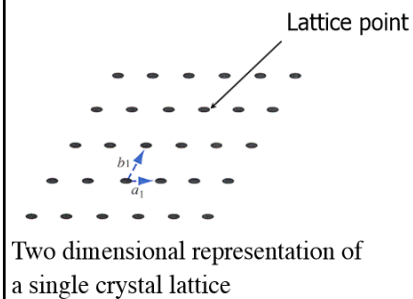
Unit Cells

- Unit cells are volumes that fill up space completely, no overlap
- A *primitive unit cell* contains exactly one Bravais lattice point; atoms in it can be used as basis to construct Xtal
- A *unit cell* can contain more than one lattice point; a *conventional unit cell* has been selected for each Bravais lattice

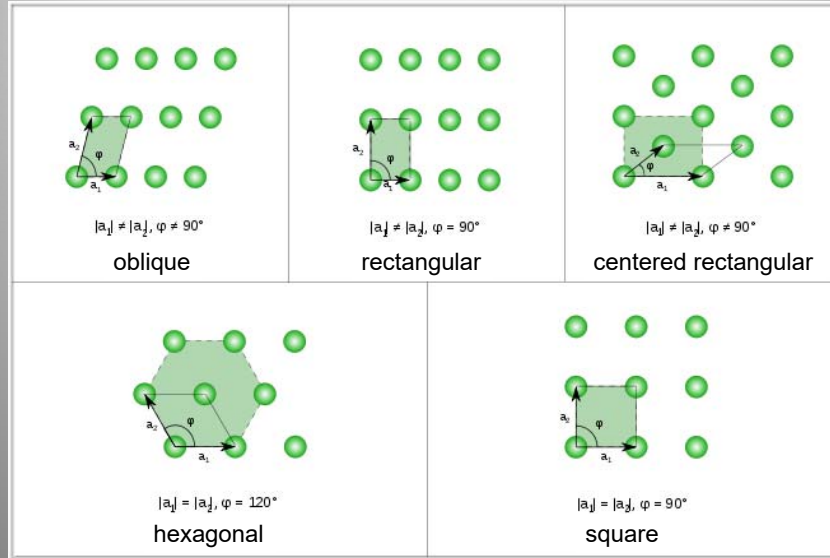


Crystalline Solids

- Example:
 - **2D oblique lattice:**
- **Basis vectors** are not necessarily orthogonal
- **Basis vectors** are not unique!

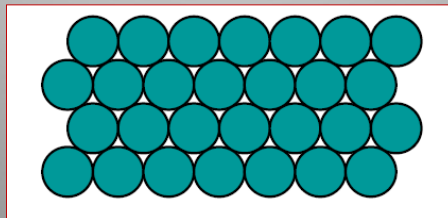


The five possible 2D crystal lattices



Example: 2D close packing of spheres

1. What is the **lattice** corresponding to this arrangement?
2. What **symmetries** does the lattice have?
3. What **axes** can be defined for this lattice?
4. What are the **primitive axes**? What is the **unit cell**?
5. How many **spheres** (circles, really! It's 2D!) are there **in a unit cell**? (Hint: add sphere fractions inside the cell.)



Example: 2D close packing of spheres

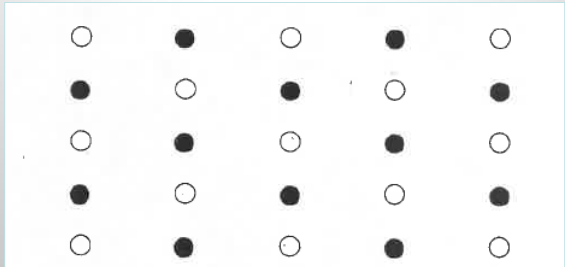
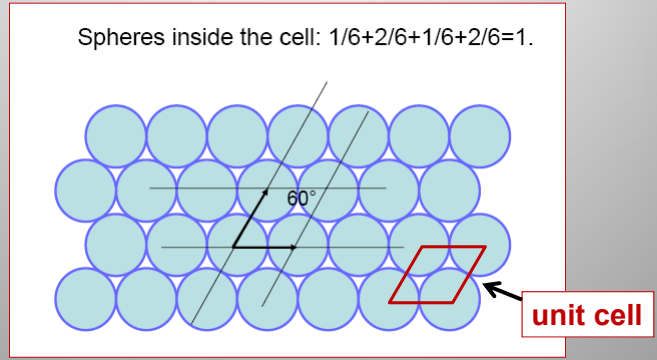


Fig. 1-22. Two-dimensional crystal for Problem 1-14.

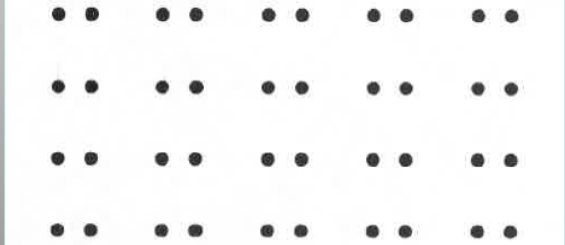
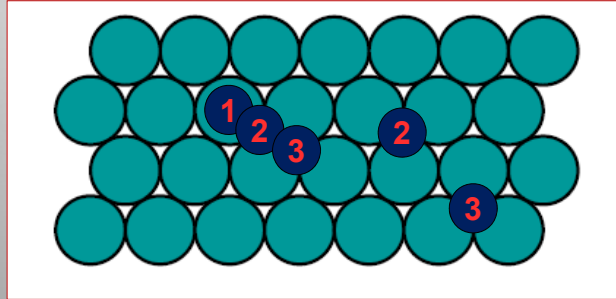


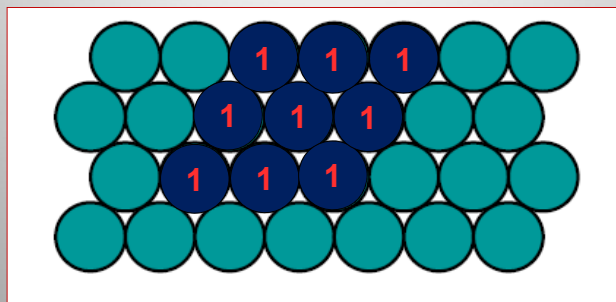
Fig. 1-23. Two-dimensional crystal for Problem 1-15.

Stacking hexagonal 2D layers to make
close packed 3D crystals



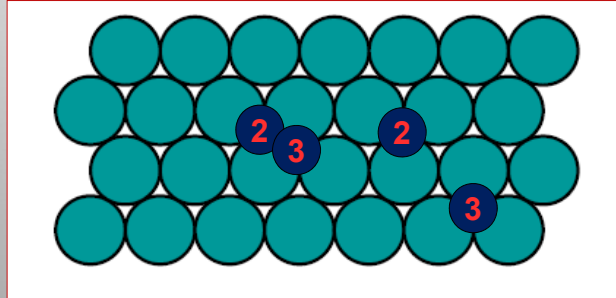
- Can stack next layer centering spheres at either point 1 or point 2 (which is same as at 3)
- Either way, each sphere has 12 nearest neighbors: 6 in its plane a, 3 above, & 3 below.

Stacking hexagonal 2D layers to make
close packed 3D crystals



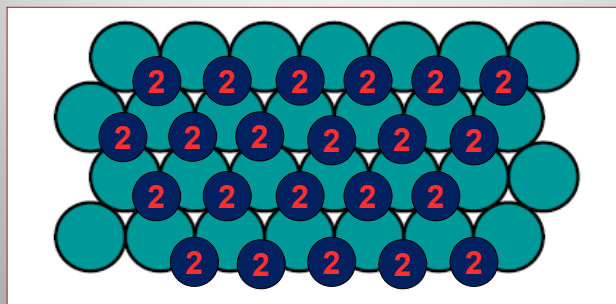
- Choosing points equivalent to point 1 does **not** result in a **close packed** structure
- Next layer would then be packed on top of these.

Stacking hexagonal 2D layers to make *close packed* 3D crystals



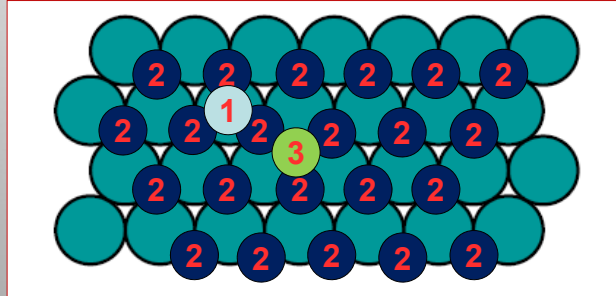
- Choosing points equivalent to point 2 or 3 does result in a *close packed* structure, with *two choices* for possible third layer ...
- [Choosing either points 2 or 3 will result in the same structure, ultimately.]

Stacking hexagonal 2D layers to make *close packed* 3D crystals



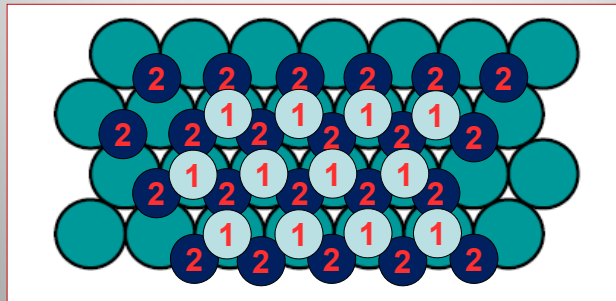
- Choosing points equivalent to point 2 or 3 does result in a *close packed* structure, with *two choices* for possible third layer ...
- [Choosing either points 2 or 3 will result in the same structure, ultimately.]

Stacking hexagonal 2D layers to make
close packed 3D crystals



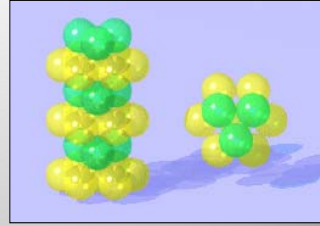
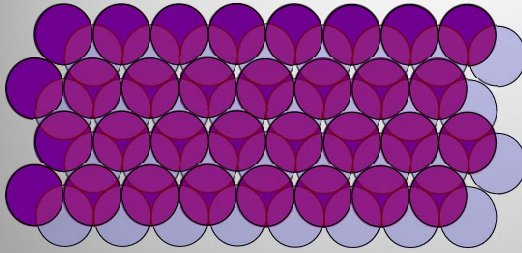
- Third layer choices: *original site 1* or *original site 3*.

Stacking hexagonal 2D layers to make
close packed 3D crystals

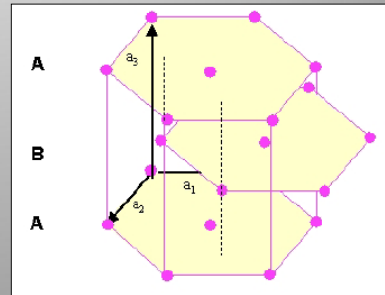


- Third layer choices: *original site 1*
- Results in **hexagonal close packed** (HCP) structure

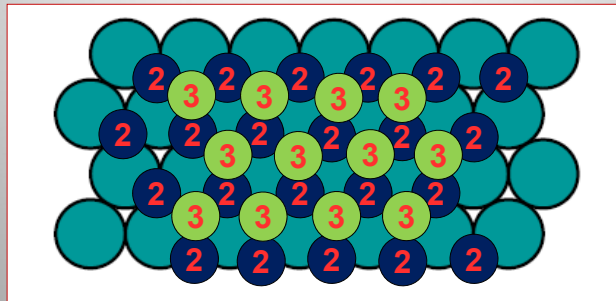
hexagonal close packed (HCP) structure



- Stacking sequence: ABABAB
- Hexagonal *Bravais* lattice with basis of two atoms

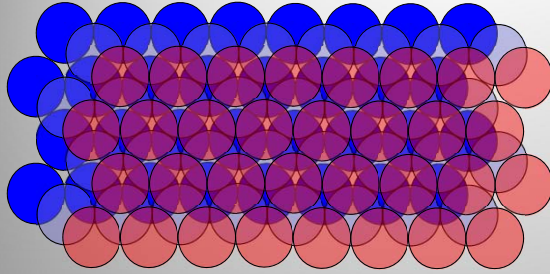


Stacking hexagonal 2D layers to make *close packed* 3D crystals

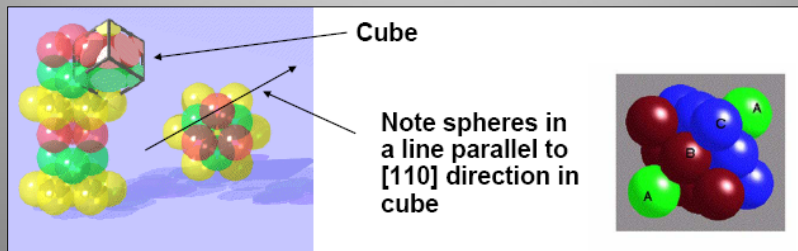


- Third layer choices: *original site 3*.
- Results in **face centered cubic** (FCC) structure

face centered cubic (FCC) structure



- Stacking sequence: ABCABCABC
- FCC Bravais lattice with basis of one atom

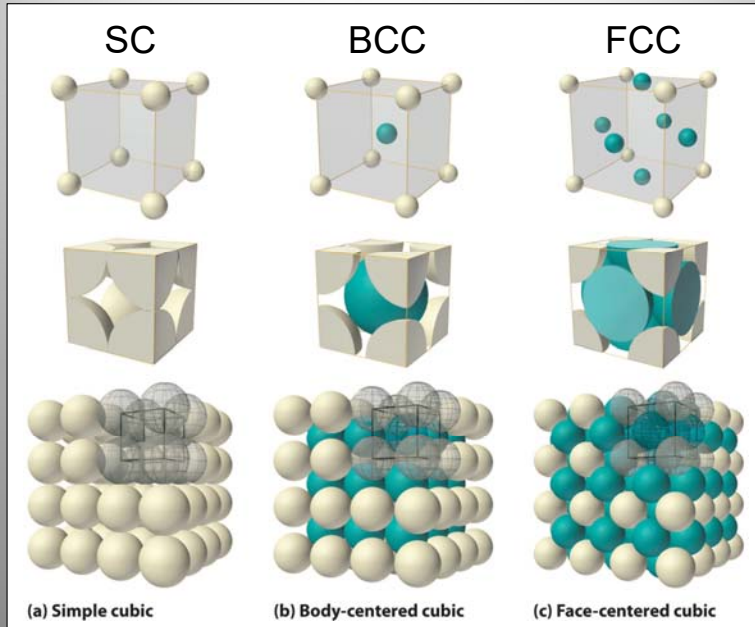


Atomium in Brussels, Belgium



Fe structure, BCC – magnified 165 billion times; Expo 1958.

Cubic lattices



Percent Ionic Character of a Single Chemical Bond

Difference in electronegativity	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5	1.6	1.7	1.8	1.9	2.0	2.1	2.2	2.3	2.4	2.5	2.6	2.7	2.8	2.9	3.0	3.1	3.2
Percent ionic character, %	1.1	1.3	1.6	2.0	2.5	3.1	3.8	4.6	5.5	6.5	7.7	9.0	10.5	12.1	13.8	15.6	17.5	19.5	21.6	23.8	26.1	28.5	31.0	33.6	36.3	39.1	42.0	45.0	48.1	51.3	54.6	58.0

DATA CONCERNING THE MOST STABLE ELEMENTARY (SUBATOMIC) PARTICLES

Symbol	Masses	Protons	Electrons*	Neutrons†	Charge
Atom (mass unit)	1.67493×10^{-27}	1.67262×10^{-27}	9.10939×10^{-31}	1.67493×10^{-27}	0
Electron (mass unit)	9.10939×10^{-31}	0	9.10939×10^{-31}	0	-1
Proton (mass unit)	1.67262×10^{-27}	1	0	0	+1
Neutron (mass unit)	1.67493×10^{-27}	0	0	1	0
Alpha particle	6.64466×10^{-27}	2	2	2	+2
Deuteron	3.34358×10^{-27}	1	1	1	+1
Triton	5.00735×10^{-27}	1	1	2	+1
Helium nucleus	6.64466×10^{-27}	2	2	2	+2

* The positive (+) or negative (-) sign to those of the proton electron or beta particle except that in alpha the negative sign (-) the antineutrino ($\bar{\nu}$) has opposite direction to those of the neutrino except that in alpha the electron is opposite to neutrino in direction of propagation.
† An antineutrino accompanies release of an electron in beta minus (β^-) particle decay, whereas a neutrino accompanies the release of a positron in β^+ decay.
‡ Together magnitudes and significant figures.

PERIODIC TABLE

The periodic table below shows the percent ionic character of a single chemical bond for various elements. The color coding indicates the percent ionic character: red (1-10%), orange (11-20%), yellow (21-30%), green (31-40%), light blue (41-50%), medium blue (51-60%), dark blue (61-70%), purple (71-80%), and black (81-90%).

KEY

- CRYSTAL STRUCTURE (SC) (BCC) (FCC)
- COVALENT RADIUS, Å
- ATOMIC RADIUS, Å
- ATOMIC VOLUME, cm³/mole
- FREE ENTHALPY OF FORMATION, kJ/mole
- POTENTIAL, V
- SPECIFIC HEAT CAPACITY, J/g °C
- THERMAL CONDUCTIVITY, W/m °C
- ELECTRONEGATIVITY (Pauling's)
- HEAT OF VAPORIZATION, kJ/mole
- HEAT OF FUSION, kJ/mole
- HEAT OF MELTING, kJ/mole
- ELECTRICAL CONDUCTIVITY, Ω⁻¹m

NOTES:

- (1) For representative oxides (higher valence) of groups 13-16. Oxides in color if color is red, blue if color is blue and semitransparent if both colors are shown. Intensity of color indicates relative strength.
- (2) Cubic, face centered; cubic, body centered; cubic.
- (3) hexagonal; rhombohedral; tetragonal; orthorhombic; monoclinic.
- (4) At 300 K (27°C).
- (5) Generality at 293 K (20°C).
- (6) From density at 300 K (27°C) for liquid and solid elements; values for gaseous elements refer to liquid state at boiling point.
- (7) Quantum mechanical value for free atom.

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