



Lecture I

Basic crystallography

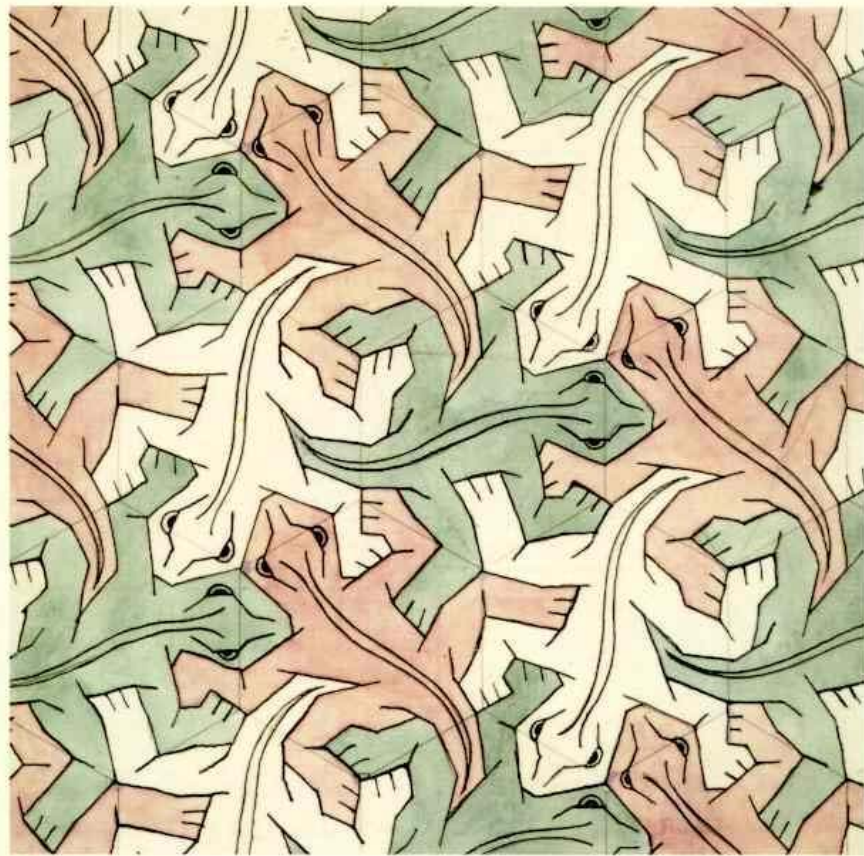
Crystals happen

basic emergent phenomenon

“ordering” of many body system

How it happens is hard to know, but one can study what happens – this is the subject of crystallography

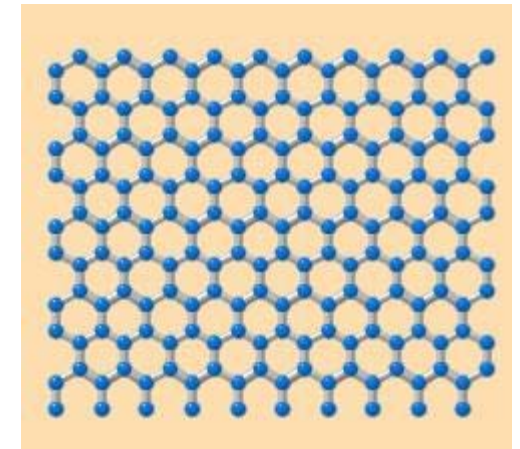
Crystal !



<http://people.via.ecp.fr/~jm/musee/escher/Lizards.jpg>

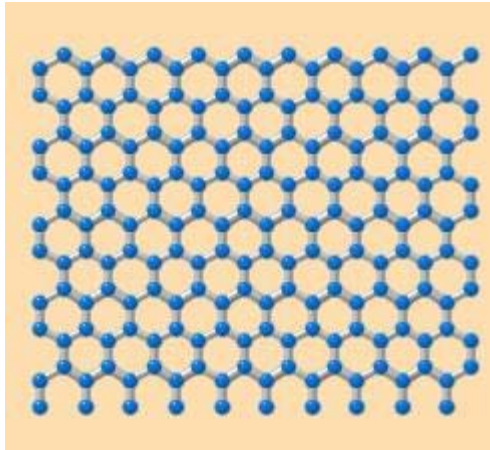
Question

- Crystal means something that repeats
Something = Basis
Repetition = **Bravais Lattice**
or Lattice in short
- How to define basis and lattice is not unique for a given crystal.
- For the graphene lattice, explain **basis**, **lattice**, and explain whether the lattice is **primitive** (i.e. basis is irreducible).



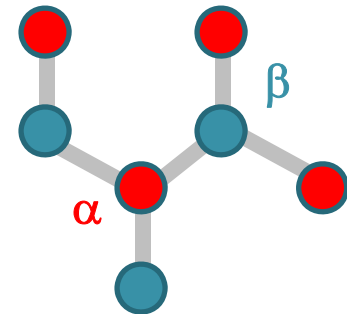
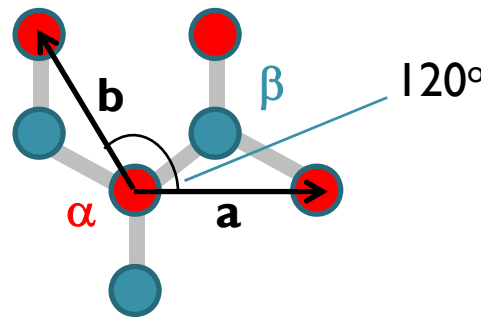
<http://www.ahwahneetech.com>

Crystal = basis and lattice



“Honeycomb” of graphene
Repeated “Benzene” ring
Each C atom is shared by three rings
Two C atoms per benzene ring
I.e. there are two C atoms per basis
Or, there are two inequivalent C atoms

<http://www.ahwahneetech.com>



Basis = α and β

Lattice = defined by unit vectors \mathbf{a} , \mathbf{b}

$|\mathbf{a}|=|\mathbf{b}|$, angle = 120° , **hexagonal (or triangular) lattice**

This lattice is a **primitive lattice**, i.e. its basis is not redundant.

Mathematically speaking ...

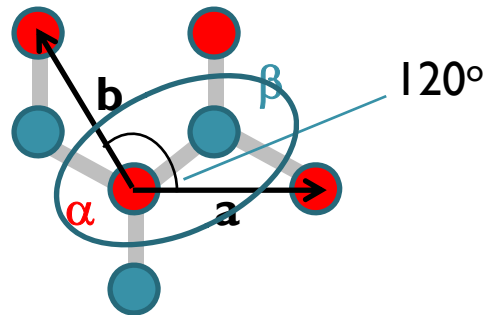
Lattice $\equiv u \mathbf{a} + v \mathbf{b}$, $u, v = \text{integers}$

(For 3d, lattice $\equiv u \mathbf{a} + v \mathbf{b} + w \mathbf{c}$, where $u, v, w = \text{integers}$)

\mathbf{a}, \mathbf{b} = unit vectors of the lattice

Basis is then specified by fractional numbers in general

Example:

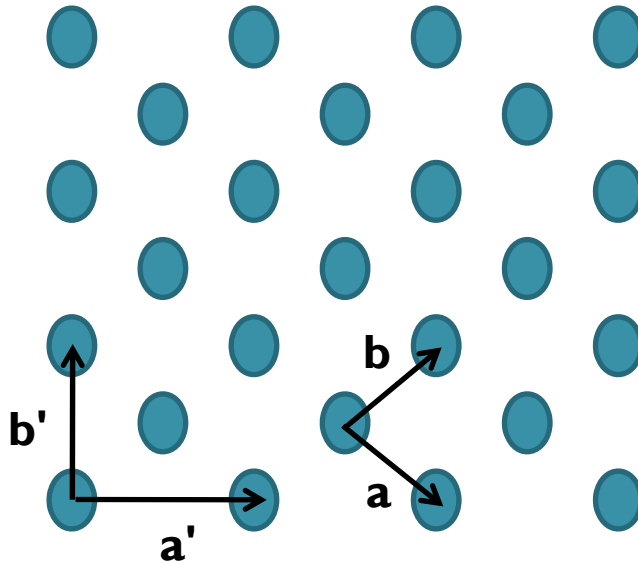


Basis coordinates:

$$0 \mathbf{a} + 0 \mathbf{b}$$

$$(2\mathbf{a} + \mathbf{b})/3$$

Crystal = basis + lattice



Centered rectangular lattice

Primitive lattice is given by,
e.g., \mathbf{a}, \mathbf{b}

$|\mathbf{a}|=|\mathbf{b}|$, angle $\neq 60^\circ, 90^\circ, 120^\circ$

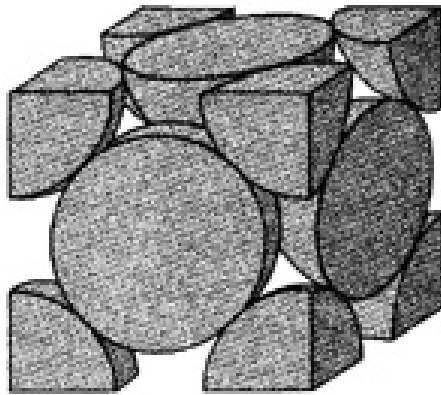
Single oval shape is the basis

Or, a lattice can be defined by
 \mathbf{a}', \mathbf{b}' and two oval shapes
(lattice is non-primitive)

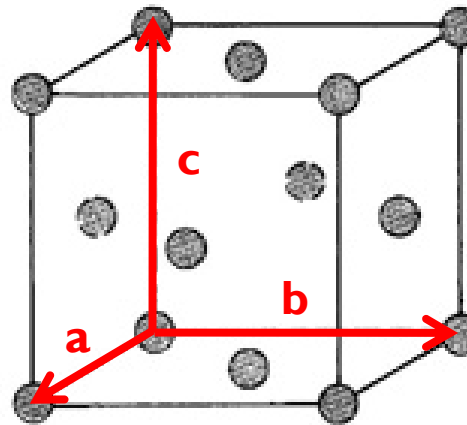
Which lattice to choose is out of convention and preference.
Often a non-primitive lattice used extensively is called a
conventional lattice.

Conventional lattice and Primitive lattice

Face Centered Cubic Lattice (fcc) or cubic closed packed (ccp) lattice



Four "atom"s per cube
(each sphere = atom)

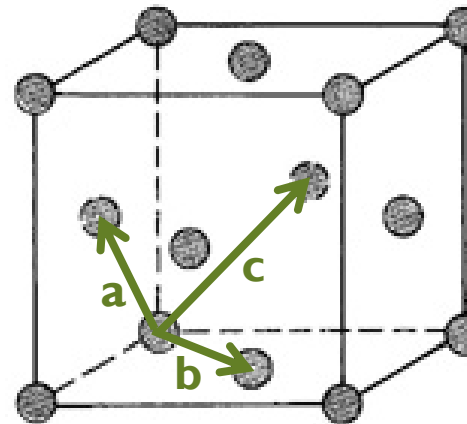


Conventional
(Cube)

$$|a| = |b| = |c|$$

All angles 90°

Four Atom Basis



Primitive
(Rhombhedron)

$$|a| = |b| = |c|$$

All angles 60°

Single Atom Basis