Lecture 1
Crystal Lattices
Position Space and Momentum Space

Crystals happen.

basic emergent phenomenon

"ordering" of many body system

It is hard to know "why" or "how."

"More is different." – P. W. Anderson

We observe them and we classify them.

Bravais Lattice

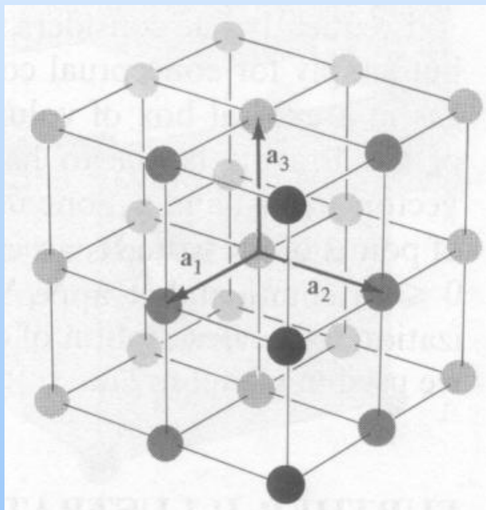
- $\mathbf{R} = n_1\, \mathbf{a}_1 + n_2\, \mathbf{a}_2 + n_3\, \mathbf{a}_3$

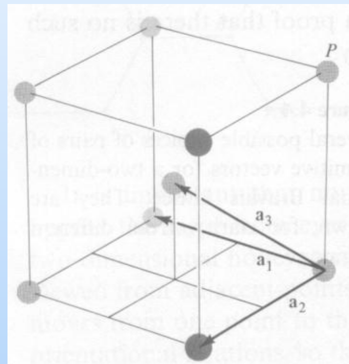
  $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$: primitive vectors

  n_1, n_2, n_3: integers
- The nature (position or momentum) of space is not specified.
- The number of primitive vectors is the same as the spatial dimension changes. I.e., the above is for 3D.

Bravais Lattice – Examples

Simple Cubic (SC)

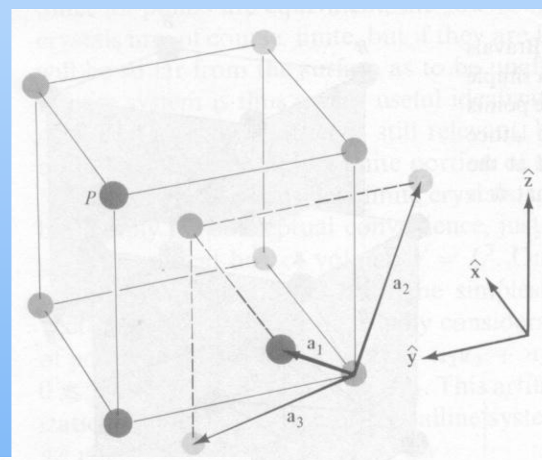


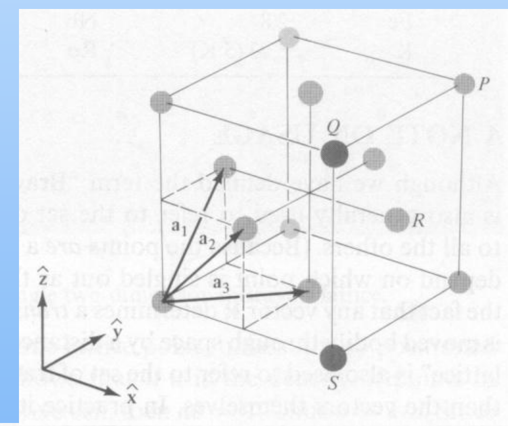


$$\mathbf{a}_1 = a\hat{\mathbf{x}}, \quad \mathbf{a}_2 = a\hat{\mathbf{y}}, \quad \mathbf{a}_3 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}}).$$

BCC

Face Centered Cubic (FCC)





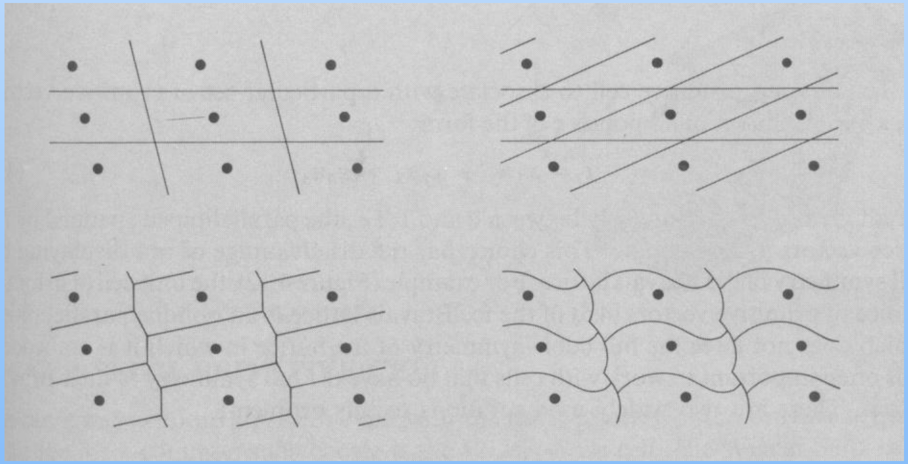
$$\mathbf{a}_1 = \frac{a}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}}), \quad \mathbf{a}_2 = \frac{a}{2}(\hat{\mathbf{z}} + \hat{\mathbf{x}}), \quad \mathbf{a}_3 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}}).$$

Body Centered Cubic (BCC)

$$\mathbf{a}_1 = \frac{a}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}} - \hat{\mathbf{x}}), \quad \mathbf{a}_2 = \frac{a}{2}(\hat{\mathbf{z}} + \hat{\mathbf{x}} - \hat{\mathbf{y}}), \quad \mathbf{a}_3 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}).$$

Unit Cell

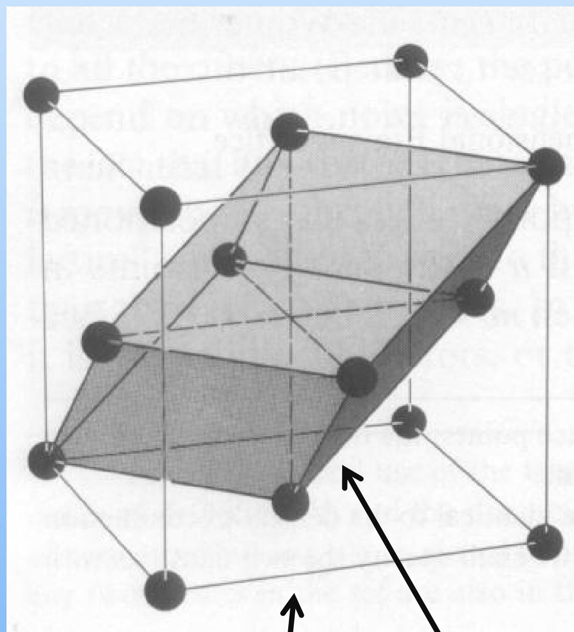
Space-filling Volume (or hyper-volume) per lattice point – can be arbitrary shape



Unit Cell – Primitive or Conventional

Primitive means "not reducible"; primitive vectors, lattice, unit cell

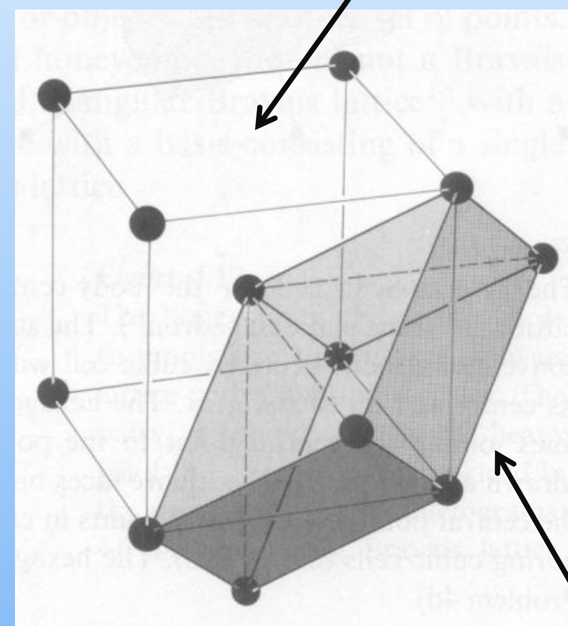
fcc



conventional

primitive

bcc

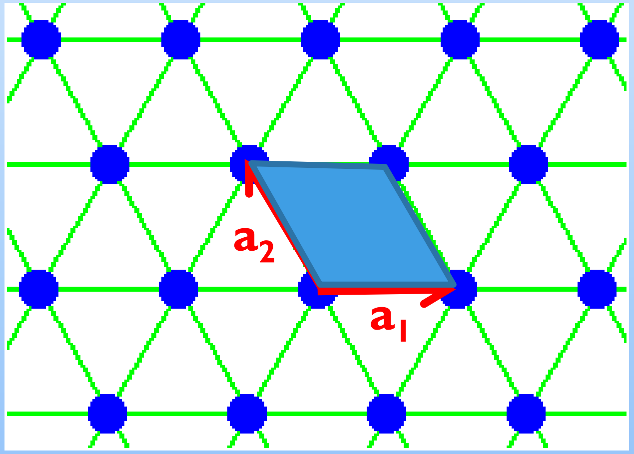


conventional

primitive

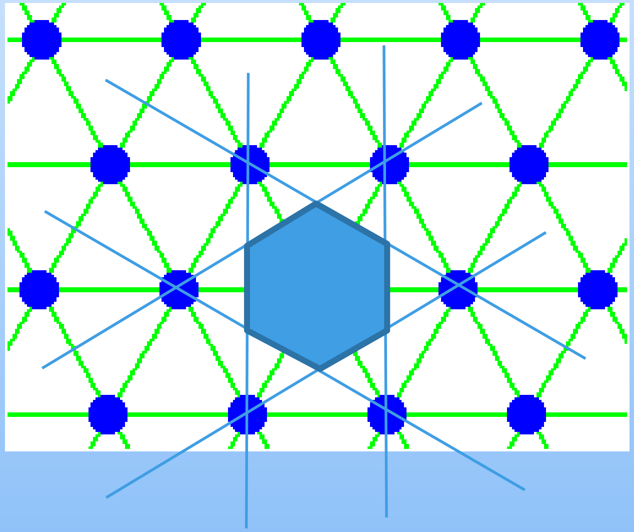
Unit Cell

Bravais Lattice (NOT crystal) of graphene



A Unit Cell

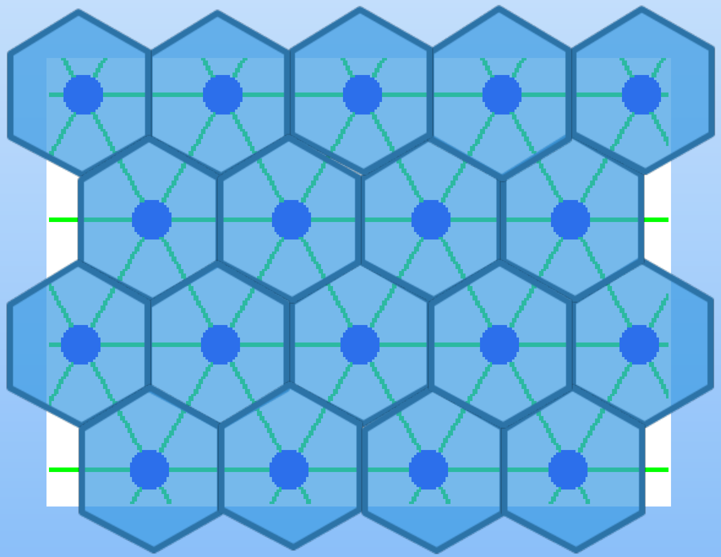
http://home.hetnet.nl/~turing/complete_hex_motif_2a.gif



Wigner Seitz Unit Cell
(Hexagon in this case)

Wigner Seitz Unit Cell

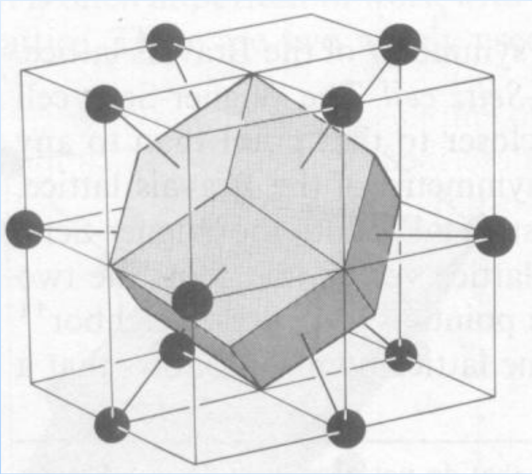
- Reflects all (point) symmetries of the Bravais lattice itself



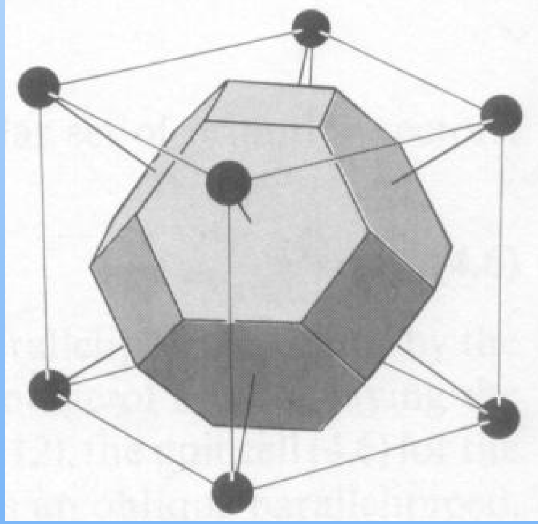
Imagine each blue ball is a balloon (or play dough) which is inflated at the same time. Eventual shape of each ball will be the WS cell – an "imprint" of its neighbors for each lattice point .

Wigner Seitz Unit Cell

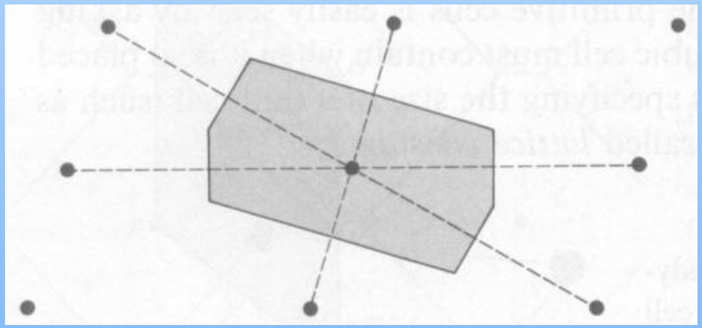
- Volume enclosed by perpendicular bi-sectors
- “Imprint” of environments
- Shows full Bravais Lattice point symmetry



fcc

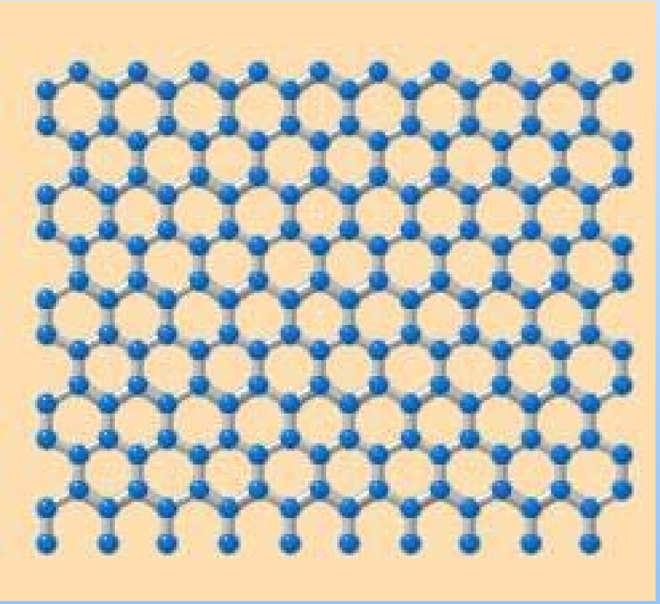


bcc



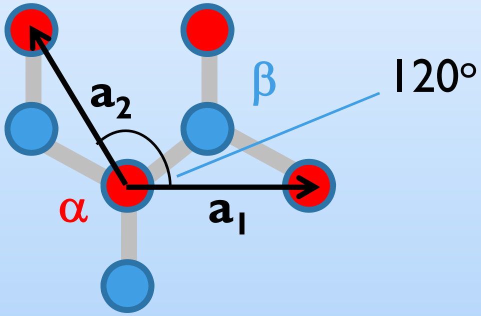
Bravais Lattice – Example in Real Crystal

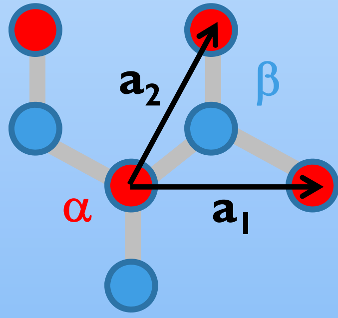
graphene



http://www.ahwahneetech.com

This honey-comb lattice is NOT a Bravais Lattice!

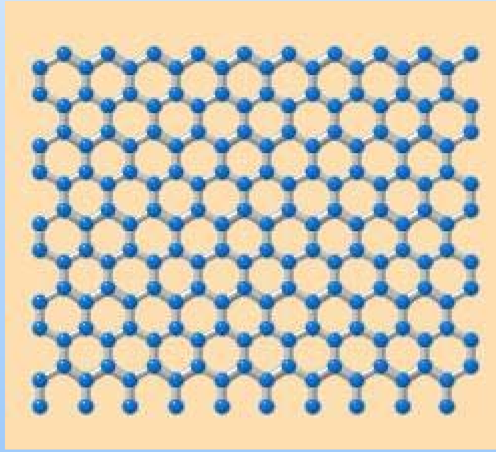




Again, primitive vectors are not unique.

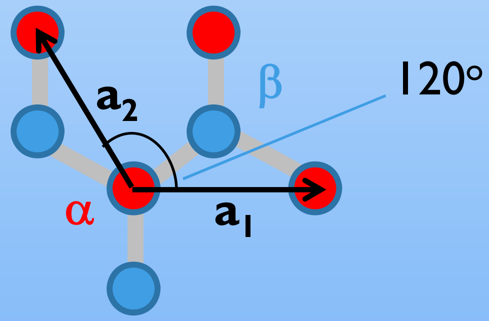
Crystal ≡ Basis + Bravais Lattice

Crystal ≡ thing that repeats



http://www.ahwahneetech.com

"Honeycomb" lattice 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



Basis = $\alpha + \beta$

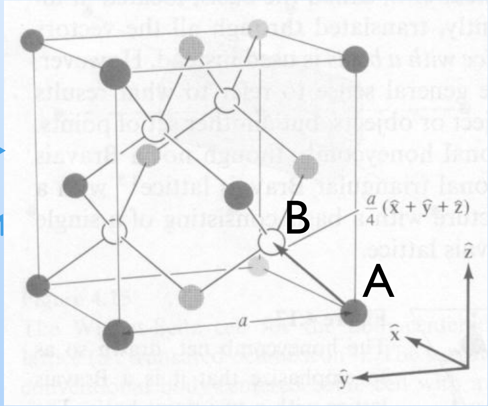
Lattice = defined by unit vectors $\mathbf{a}_1$, $\mathbf{a}_2$

$|\mathbf{a}_1| = |\mathbf{a}_2|$, angle = 120°, **hexagonal (or triangular) lattice**

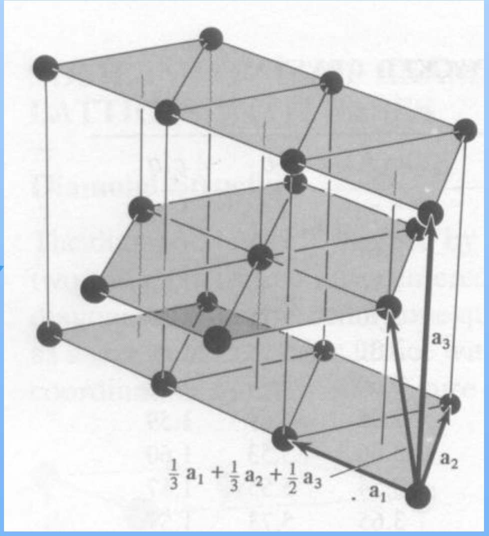
This lattice is a **primitive lattice**, i.e. its basis is not reducible to a smaller basis.

Examples of Crystal Structures

- Diamond Structure
  (fcc + 2 identical atom basis; A=B)
- Zinc-Blend Structure
  (fcc + 2 different atom basis; A≠B)

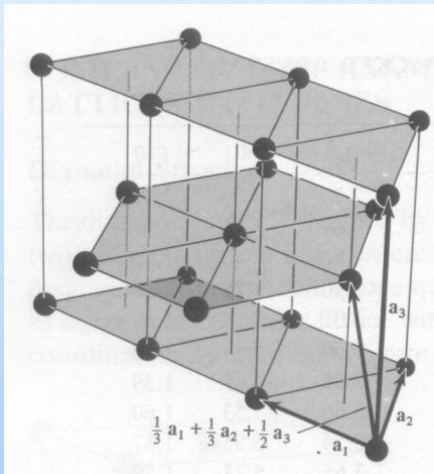


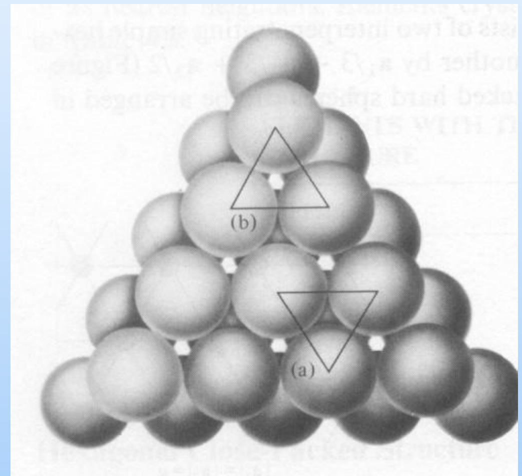
- Hexagonal Close Packed Structure (hcp)
  (hexagonal lattice + 2 identical atom basis)



Close-Packed Structures

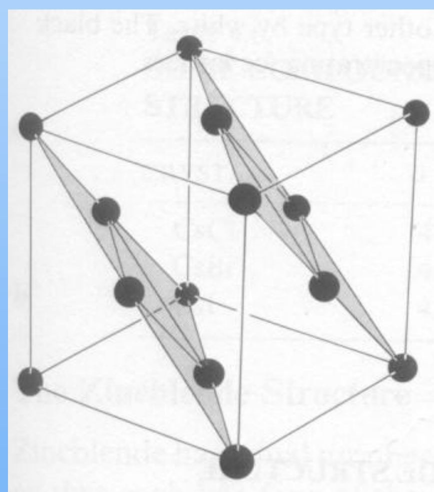
- hcp

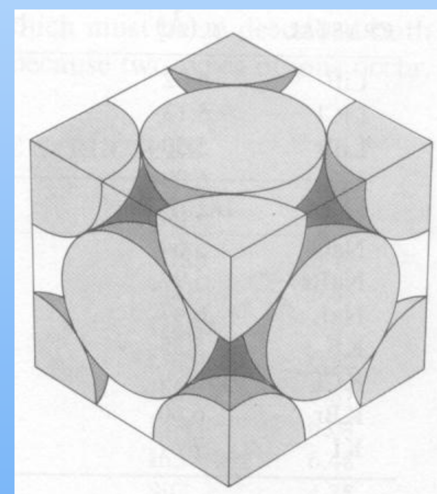




AB-AB packing of “marbles”

- fcc





ABC-ABC packing of “marbles”

Reciprocal Lattice

- Bravais Lattice applies to any space – position space ("real" space, as commonly called) or momentum space
- Position space and momentum space are <u>reciprocals</u> of each other – sort of like Fourier transform pairs

Reciprocal Lattice – Definition

- $\mathbf{b}_i \cdot \mathbf{a}_j \equiv 2\pi\, \delta_{ij}$
- The Bravais lattice formed by $\{\mathbf{b}_i\}$ is the reciprocal lattice of the BL formed by $\{\mathbf{a}_i\}$.
- The reciprocal of the reciprocal is self.
- For $\mathbf{R} = n_1\, \mathbf{a_1} + n_2\, \mathbf{a_2} + n_3\, \mathbf{a_3}$ (n: integer) and $\mathbf{K} = m_1\, \mathbf{b_1} + m_2\, \mathbf{b_2} + m_3\, \mathbf{b_3}$ (m: integer) $\exp(i\, \mathbf{K} \cdot \mathbf{R}) = 1$ for any m's and n's (plane wave with the periodicity of the lattice)
- Usual notation:
  real space **a**, momentum space **a***

Reciprocal Lattice – Construction

- In 3 dimensions

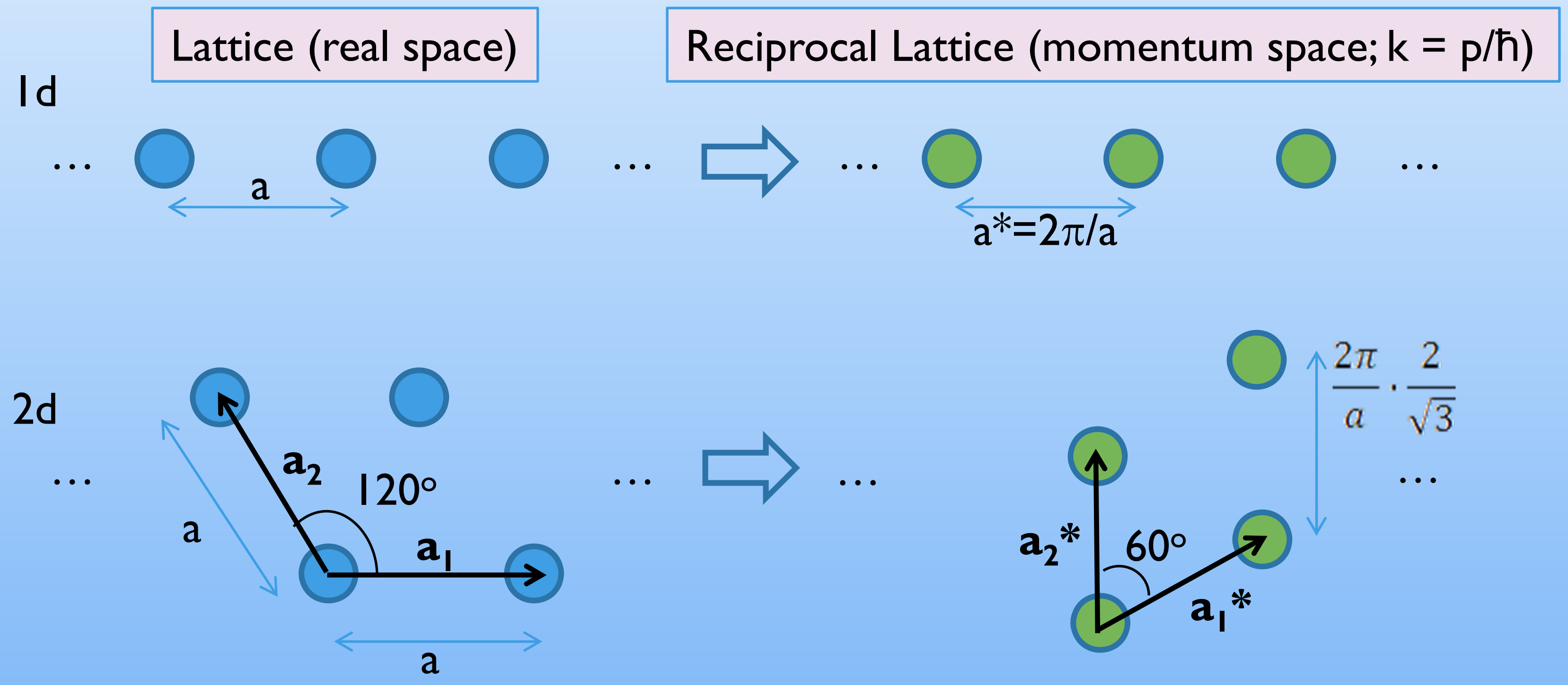
$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)},$$

$$\mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)},$$

$$\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}.$$

- In 2 dimensions, send one of a's to infinity, or do the geometry on paper.
- In 1 dimension, it is trivial, $b = 2\pi/a$.

Reciprocal Lattice – Construction



More about Reciprocal Lattice

- V = volume of unit cell

  V* = volume of reciprocal unit cell

  $VV^* = (2\pi)^d$ (d = dimension, 1, 2, 3 (>= 4 ?!))
- Reciprocal of fcc is bcc and vice versa

  Reciprocal of hexagonal is hexagonal
- [First] <u>**Brillouin zone**</u> ≡ Wigner Seitz Cell of the momentum (i.e. wave vector) space