Phys 412 Solid State Physics

Lecturer: Réka Albert

Physics 412 Solid State Physics
Fall 2006

Instructor: Réka Albert
Office: 122 Davey, office hours Monday 1-4 pm
Phone: 865-6123

Meeting time and place:

- Monday, Wednesday 9:05-9:55 am, 104 Osmond
- Friday 9:05-9:55 am, 313 Osmond

Texts:

- C. Kittel, Introduction to Solid State Physics (Wiley, 8th Edition)
- R. H. Silsbee and J. Dräger, Simulations for Solid State Physics (Cambridge, 1997)
  Software downloadable from http://www.physics.cornell.edu/sss/download.html

Topics:

- Crystal structure
- Reciprocal lattice
- Crystal binding
- Phonons
- Free electron Fermi gas
- Energy bands
- Ferromagnetism and Ising model

Grading:

- 3 exams, 15% each (total 45%)
- 8 homework assignments, 2.5% each (total 20%)
- 6 simulation reports, 2.5% each (total 15%)
- 1 term project, 20%

Exams: The exams will be take-home, open-book exams. They will be handed out at the end of the class period on Oct 4, Nov. 1 and Dec. 1 and will be due at the beginning of the class period on the following class. These exams are to be done individually -you may not discuss them with anyone except me until after they are turned in. The exams will be designed to take about 1-2 hours, but you may spend longer - just be sure to hand them in on time. Each exam will contribute 15% to the final grade.

Homework 8 homeworks will be assigned and will be due on the days specified in the syllabus. Homework problems selected from the main textbook (Kittel) will be combined with questions based on previously performed simulations. The homework will be graded on a 1-5 scale; each homework grade will contribute 2.5% of the final grade.

Simulation reports A "lab" sheet with questions and exercises (based on the Solid State Simulation textbook) will be given out for each simulation chapter (6 total). The sheets will be completed during Friday's class and will be due at the end of class on the days specified in the syllabus. The reports will be graded on a 1-3 scale; each grade will contribute 2.5% of the final grade.

Term Project The project should be an in-depth study of one topic or an aspect of a topic in solid state physics. The goal is to obtain a deep understanding of one issue in solid state physics, and to explain that issue in a short presentation and a paper which can be understood by your fellow students. Project topics will be chosen by the students by the end of Thanksgiving break. Students will give a 10 minute presentation on their projects during the last week of classes. A project report of about 5 pages will be due on December 15. The presentations and reports will be graded for content and clarity and will contribute a total of 20% of the final grade.

Academic Integrity

All Penn State policies regarding ethics and honorable behavior apply to this course. Academic dishonesty includes, but is not limited to, cheating, plagiarizing, fabricating of information or citations, facilitating acts of academic dishonesty by others, having unauthorized possession of examinations, submitting work of another person or work previously used without informing the instructor, or tampering with the academic work of other students. For any material or ideas obtained from other sources, such as the text or things you see on the web, in the library, etc., a source reference must be given. Direct quotes from any source must be identified as such. All exam answers must be your own, and you must not provide any assistance to other students during exams. Any instances of academic dishonesty WILL be pursued under the University and Eberly College of Science regulations concerning academic integrity.

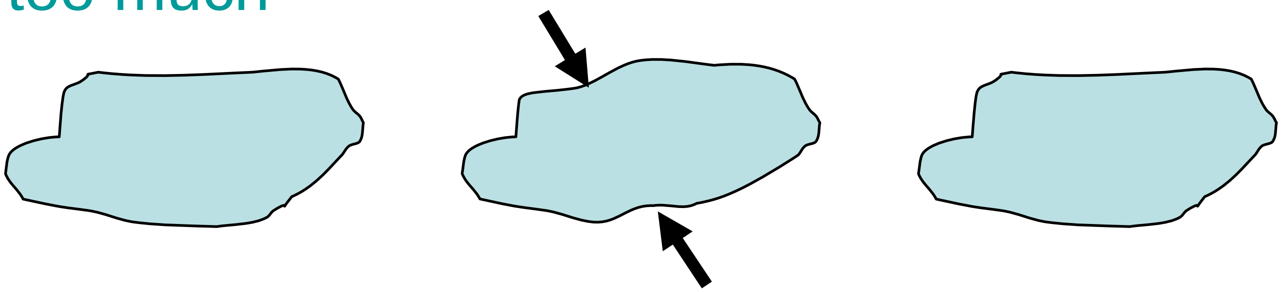
Assigned Exercises in Solid State Simulations

- Bravais: 1, 3-6, 8, 9, 11, 12, 17, 21, 25, 26
- Laue: 3, 4, 8, 10, 19, 23, 34, 37
- Born: 2, 4-10, 15, 17, 22, 23-25, 27-30
- Debye: 7-9, 12, 14, 16, 17, 19, 22, 28-30, 34, 35
- Drude: 1, 2, 4, 5, 7, 10, 22-24, 30
- Ising: 1-4, 13, 15

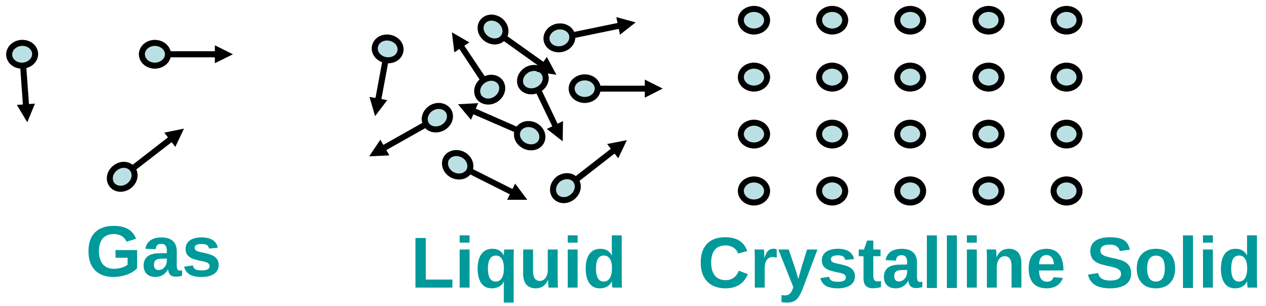
Week	Date	Monday	Wednesday	Friday
1	9/04	Labor Day	Chapter 1 - lattices	SSS Bravais
2	9/11	Chapter 1 - planes	Chapter 1 - structures	SSS Bravais
3	9/18	Chapter 2 - reciprocal space	Chapter 2 - diffraction HW 1 due	SSS - Bravais, Laue Bravais report due
4	9/25	Chapter 2 - diffraction	Chapter 3 - interactions HW 2 due	SSS - Laue Laue report due
5	10/02	Chapter 3 - interactions	Review of Ch. 1-3 HW 3 due	No class
6	10/09	Chapter 4 - vibrations Exam 1 - Ch 1-3 handed out	Chapter 4 - vibrations Exam 1 collected	SSS - Born
7	10/16	Chapter 4 - vibrations	Chapter 5 - phonons HW 4 due	SSS - Born
8	10/23	Chapter 5 - phonons	Chapter 5 - phonons HW 5 due	SSS - Born Born report due
9	10/30	Chapter 5 - phonons	Review of Ch. 4,5 HW 6 due	SSS - Debye
10	11/06	Chapter 6 - free electrons Exam 2 - Ch 4,5 handed out	Chapter 6 - free electrons Exam 2 collected	SSS - Debye
11	11/13	Chapter 6 - free electrons	Chapter 6 - free electrons HW 7 due	SSS - Debye Debye report due
12	11/20	Chapter 7 - energy bands	SSS - Drude (Tuesday)	Thanksgiving
13	11/27	Chapter 7 - energy bands HW 8 due	Chapter 7 - energy bands	SSS - Drude Drude report due
14	12/04	Review of Ch 6.7 Exam 3 - Ch 6,7 handed out	Ferromagnetism Exam 3 collected	SSS - Ising Ising report due
15	12/11	Project presentations	Project presentations	Papers due by 5pm in 122 Davey

What is a solid?

- A material that keeps its shape
  - Can be deformed by stress
  - Returns to original shape if it is not strained too much



  - Solid structure is defined by the atoms



What is Solid State Physics?

- The body of knowledge about the fundamental phenomena and classifications of solids
- “fundamental phenomenon” = a characteristic behavior exhibited by classes of solids
- Examples:
  - Ductile vs. brittle materials
  - Metals vs. Insulators
  - Superconductivity - discovered in 1911
  - Ferromagnetic materials
- The basic understanding of such “fundamental phenomena” has only occurred in the last 70 years - due to quantum mechanics

Phenomena and Principles in SSP

- Mechanical
  - Structures
  - Strength
- Thermal
  - Heat capacity
  - Heat conduction
  - Phase transitions
- Electrical
  - Insulators
  - Metals
  - Semiconductors
  - Superconductors
- Magnetic
  - Ferromagnetism
- Optical
  - Reflection, refraction
  - Colors

↔

- Newton’s Laws
- Maxwell’s Equations
- Thermodynamics and Statistical Mechanics
- Quantum Mechanics
  - Schrodinger’s Equation
  - Pauli exclusion principle
- Order and Symmetry

Course outline

- Structures of solids: Kittel 1-5
  - crystal structure
  - diffraction and reciprocal lattice
  - binding
  - atomic vibrations and elastic constants
  - thermal properties
- Electronic properties: Kittel 6-7
  - free electron gas
  - energy bands – metals vs. insulators
  - semiconductors (time permitting)
- Additional topics (time permitting)

Solid State Simulations

- “bravais”: Crystal structure and x-ray diffraction
- “laue”: Diffraction in perfect and imperfect crystals
- “born”: Lattice dynamics in one dimension
- “debye”: Lattice dynamics and heat capacity
- “drude”: Dynamics of the classical free electron gas
- “ising”: Ising model and ferromagnetism

Structure of Crystals (Kittel Ch. 1)

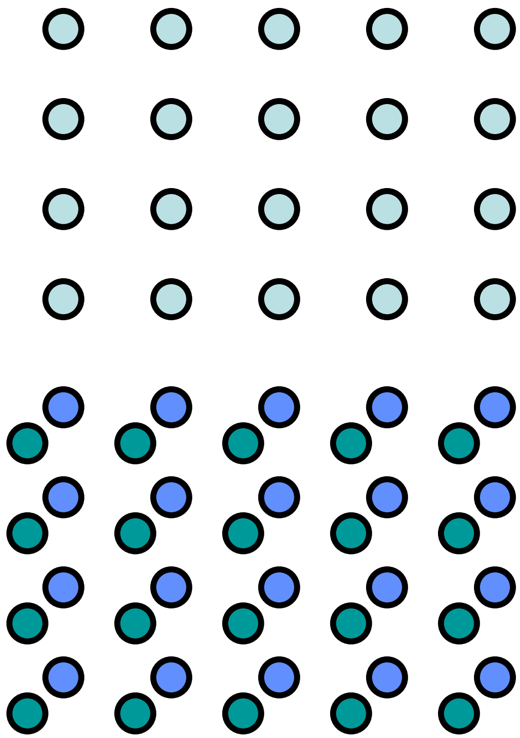
A crystal is a repeated array of atoms.

See many great sites like "Bob's rock shop" with pictures and crystallography info: **http://www.rockhounds.com/rockshop/xtal/index.html**

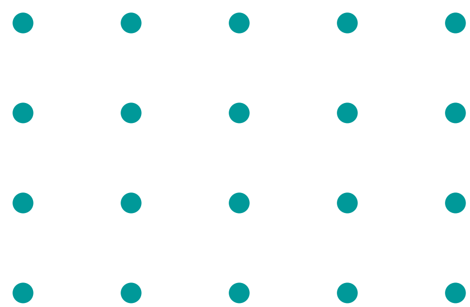
Crystals

- A crystal is a repeated array of atoms (or cells)

- Crystal = Lattice + Basis



Crystal

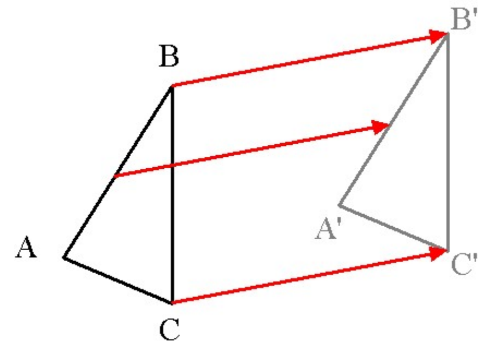


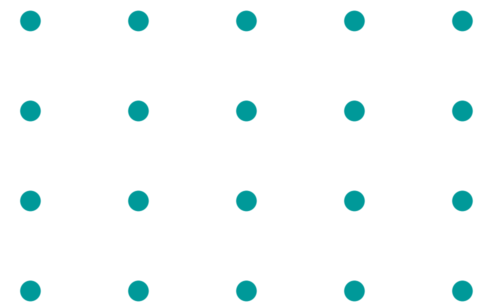
Lattice of points
(Bravais Lattice)

Basis of atoms

Possible crystal symmetries

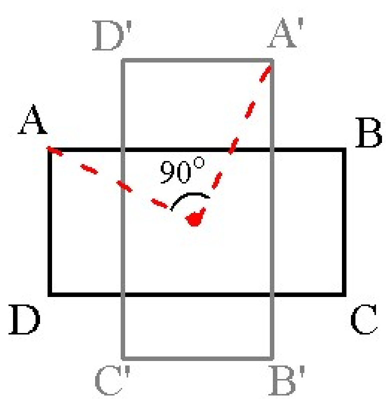
- Translation symmetry

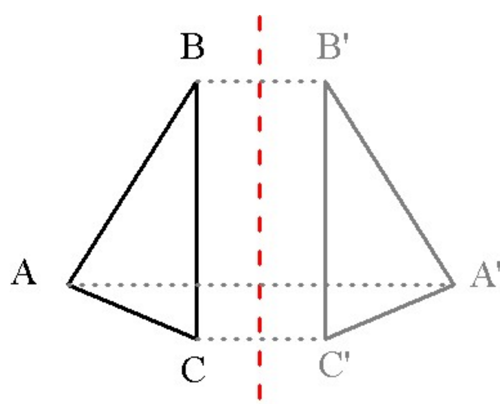


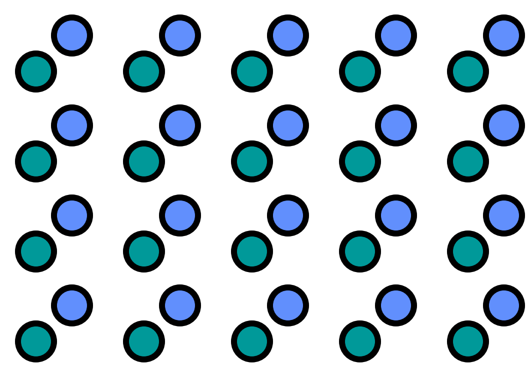


always present

- Point symmetries (rotation, reflection)







depend on basis

Characterizing the lattice

Each lattice has translational symmetry - the atomic arrangement looks the same when viewed from the lattice point at **r** or from the lattice point at

$$\boldsymbol{r}' = \boldsymbol{r} + u_1 \boldsymbol{a_1} + u_2 \boldsymbol{a_2} + u_3 \boldsymbol{a_3}$$

$\mathbf{a_1}$, $\mathbf{a_2}$, $\mathbf{a_3}$ **-** translation vectors (axes), only 2 needed in 2D
where u_1 , u_2 , u_3 are arbitrary integers

There are multiple ways of choosing axes. Each choice determines a unit cell; the crystal is the repetition of these unit cells.

Primitive axes:

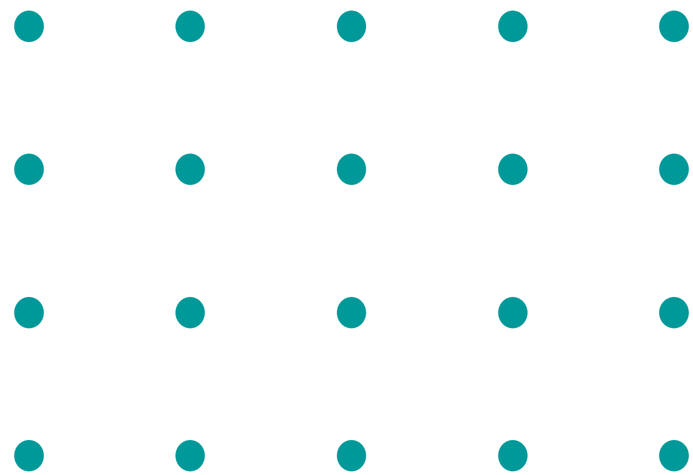
– each point of the lattice can be described as $u_1 \boldsymbol{a_1} + u_2 \boldsymbol{a_2} + u_3 \boldsymbol{a_3}$
– the parallelepiped defined by them has the smallest volume

The primitive translation vectors determine the primitive cell.
There are many ways of choosing primitive axes, but there is always one lattice point (and as many atoms as there are in the basis) per primitive cell.

Ex. Define a few possible sets of axes for the lattice below.

Which are the primitive axes?

What is the primitive cell?



Characterizing the basis

A basis of atoms is attached to every lattice point, with every basis identical

Coordinates of atoms in the basis

$$\boldsymbol{r_j} = x_j \boldsymbol{a_1} + y_j \boldsymbol{a_2} + z_j \boldsymbol{a_3}$$

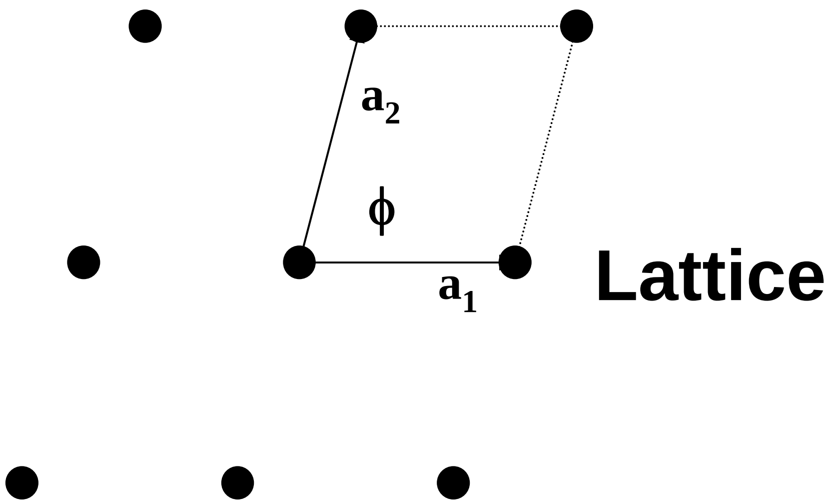
$\mathbf{a_1}$, $\mathbf{a_2}$, $\mathbf{a_3}$ - lattice axes

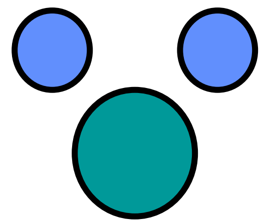
x_j, y_j , z_j are between 0 and 1

Description of a crystal:

1. What is the lattice?
2. What choice of $\mathbf{a_1}$, $\mathbf{a_2}$, $\mathbf{a_3}$ do we wish to make?
3. What is the basis?

Two Dimensional Crystals



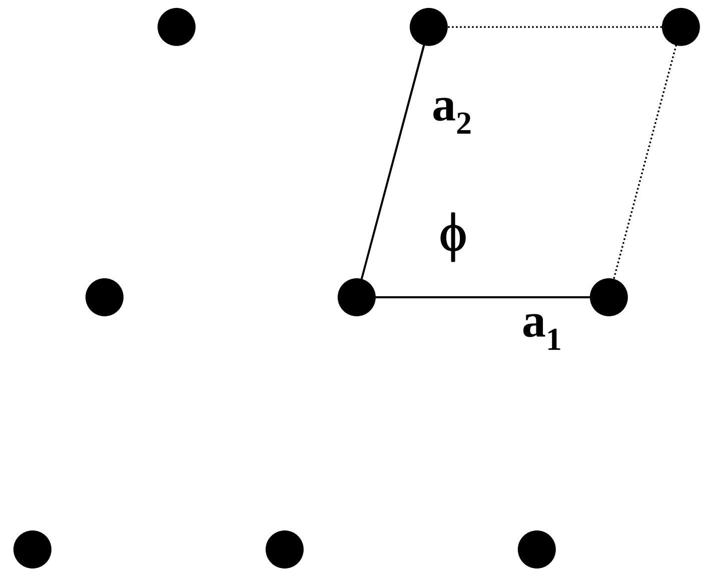


- Infinite number of possible crystals
- Finite number of possible crystal types (Bravais lattices)
- The entire infinite lattice is specified by the primitive vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ (also $\mathbf{a}_3$ in 3D)

Wallpaper patterns as crystals

Find the lattice and basis of these two wallpaper patterns.
What symmetries do the patterns have?

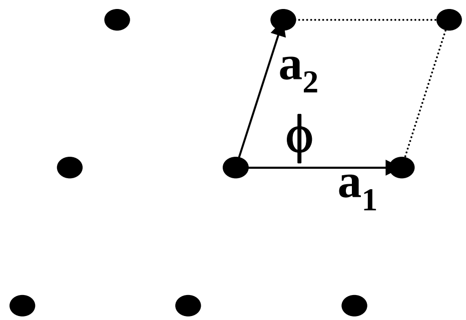
Possible Two Dimensional Lattices



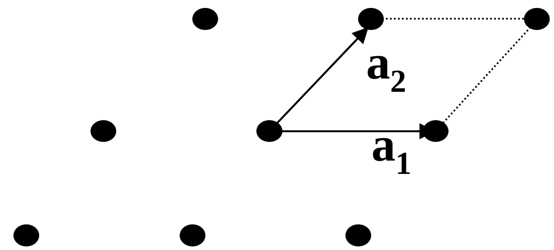
- Special angles ϕ = 90° and 60° lead to special crystal types
- In addition to translations, these lattices are invariant under rotations and/or reflections

- Ex: give a few examples of lattices with ϕ = 90° or ϕ = 60°:

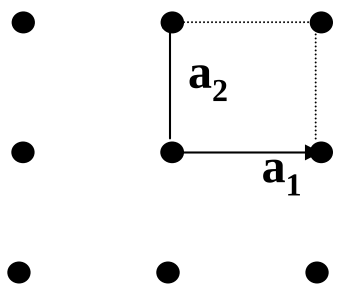
Possible Two Dimensional Lattices



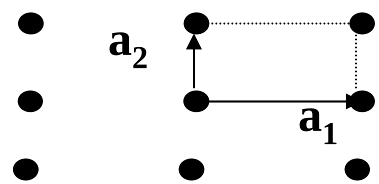
General oblique



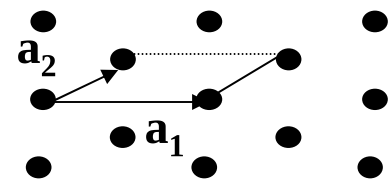
Hexagonal $\Phi = 60$, $a_1 = a_2$
6-fold rotation , reflections



Square
4-fold rot., reflect.



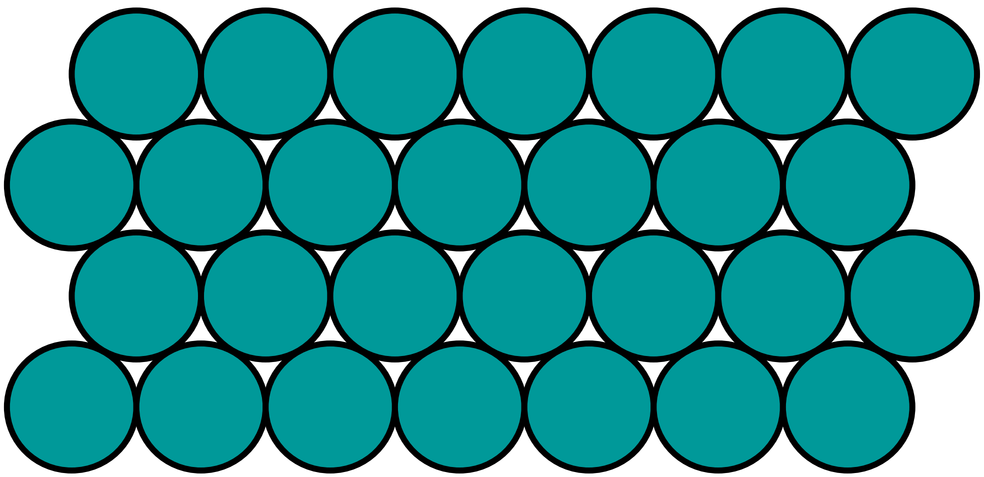
Rectangular
2-fold rot., reflect.



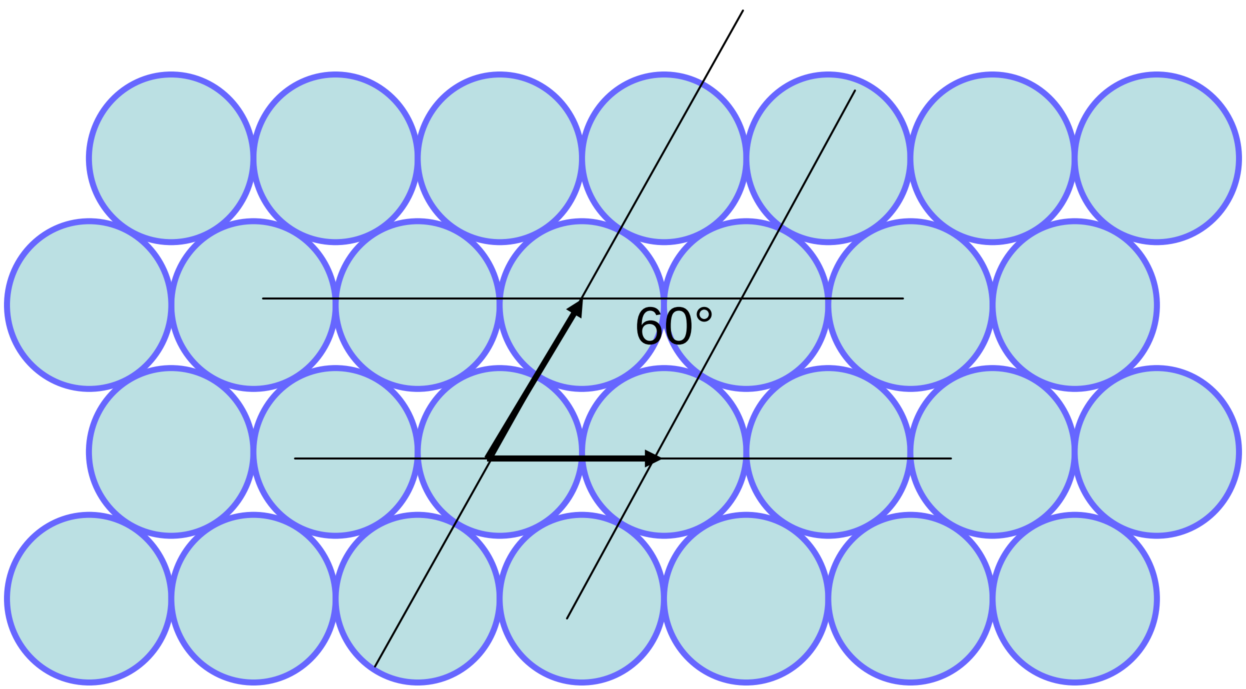
Centered Rectangular
2-fold rot., reflect.

These are the only possible special crystal types (Bravais lattices) in two dimensions.

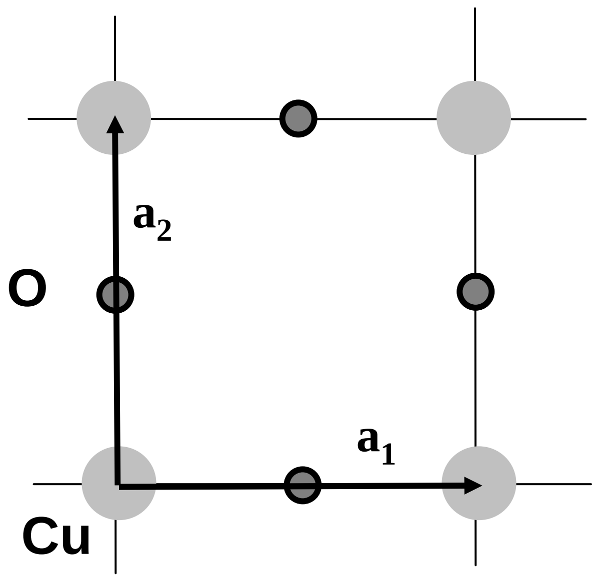
Ex.: Close packing of spheres
What is the lattice corresponding to this arrangement?
What symmetries does the lattice have?
What axes can be defined for this lattice?
What are the primitive axes?
How many spheres are there in a cell? Hint: add sphere fractions inside the cell.



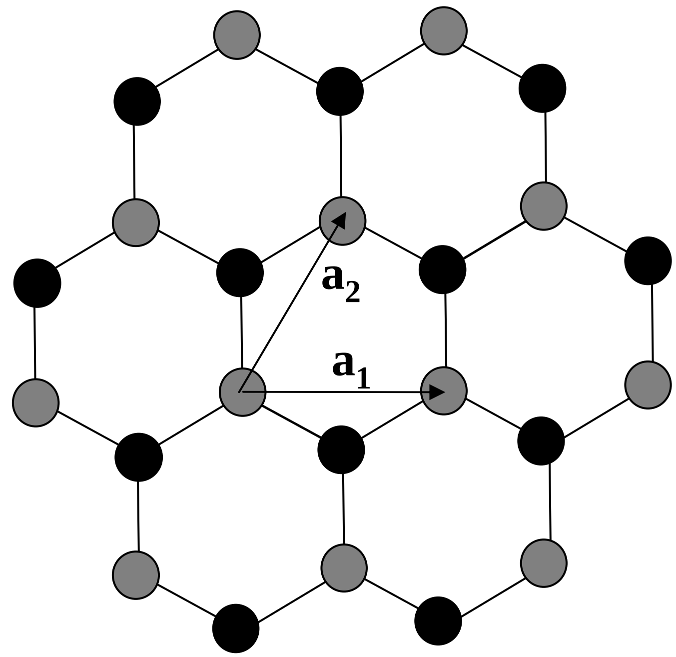
Spheres inside the cell: 1/6+2/6+1/6+2/6=1.



Crystalline layers with >1 atom basis



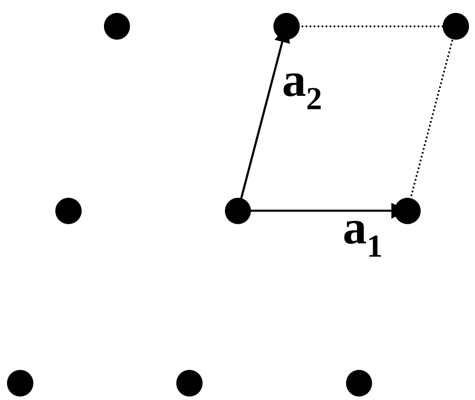
CuO_2 Square Lattice



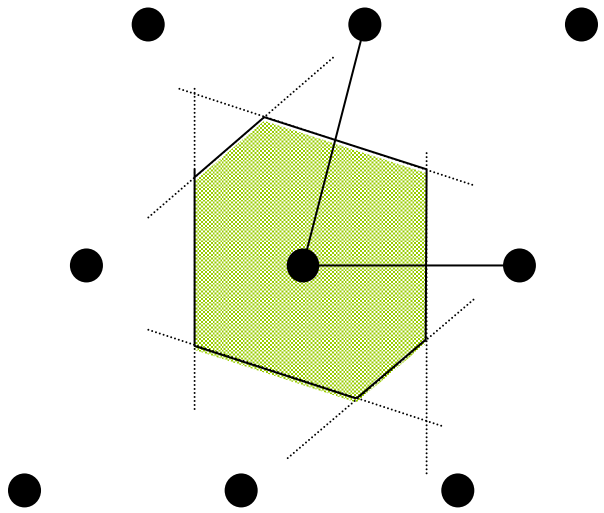
Honeycomb Lattice
(Graphite or BN layer)

- Left - layers in the High T_c superconductors
- Right - single layer of carbon graphite or hexagonal BN (the two atoms are chemically different in BN, not in C)

Primitive Cell and Wigner-Seitz Cell



One possible Primitive Cell



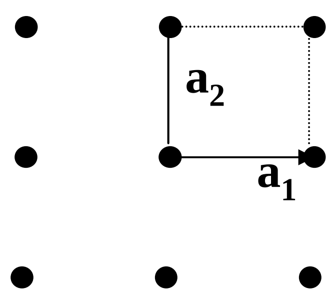
Wigner-Seitz Cell -- Unique

Wigner Seitz Cell is most compact, highest symmetry primitive cell possible

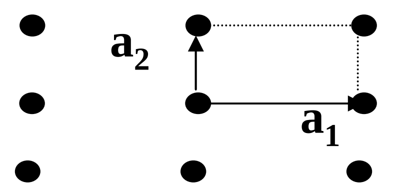
It is defined by the neighboring lattice points:

- connect a lattice point to all nearby lattice points
- draw the perpendicular bisectors of lines
- find enclosed polygon with smallest volume

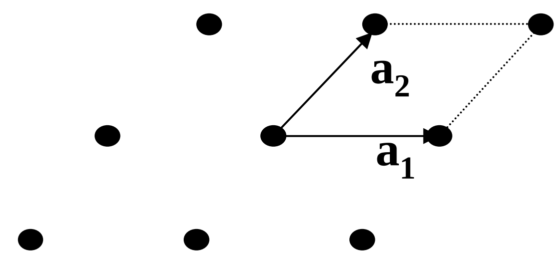
Ex. Find the Wigner-Seitz cell of the following lattices



Square
4-fold rot., reflect.

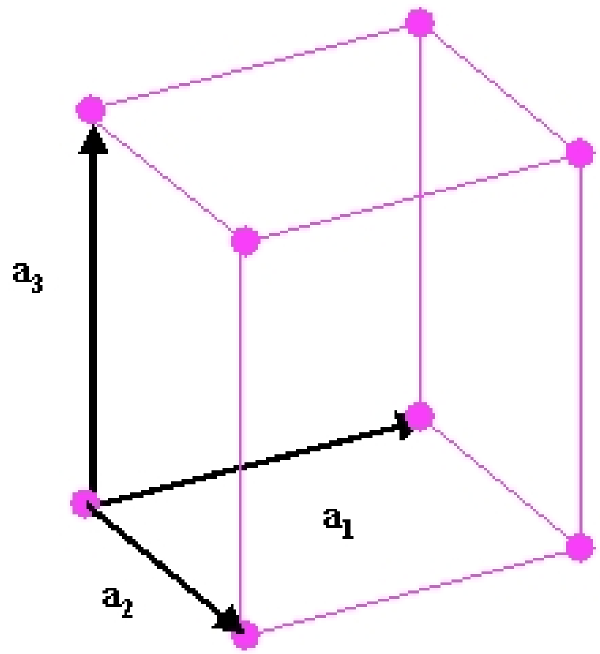


Rectangular
2-fold rot., reflect.

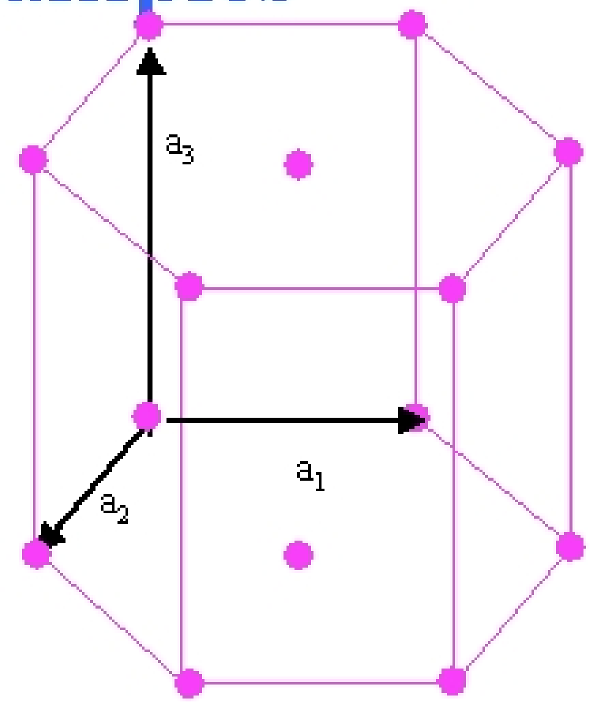


Hexagonal $\Phi = 60$, $a_1 = a_2$
6-fold rotation , reflections

Three Dimensional Lattices
Simplest examples



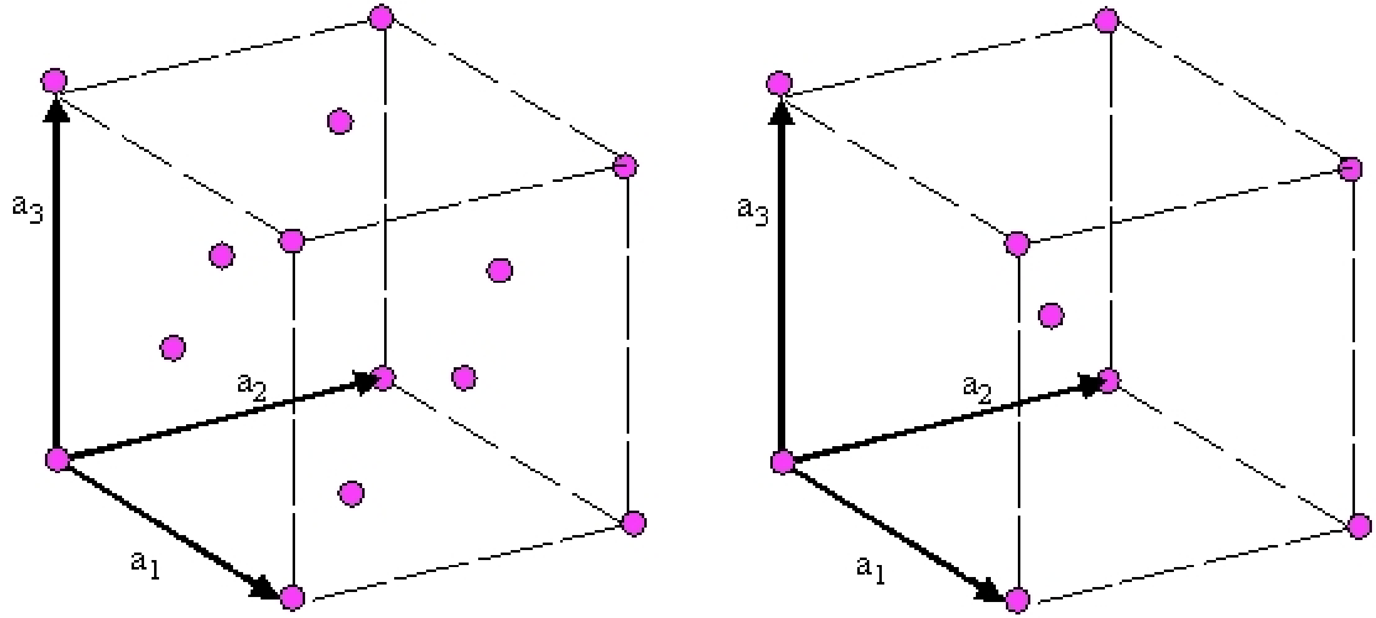
Simple Orthorhombic Bravais Lattice



Hexagonal Bravais Lattice

- **Orthorhombic: angles 90 degrees, 3 lengths different**
  Tetragonal: 2 lengths same; Cubic: 3 lengths same
- **Hexagonal: a_3 different from a_1, a_2 by symmetry**

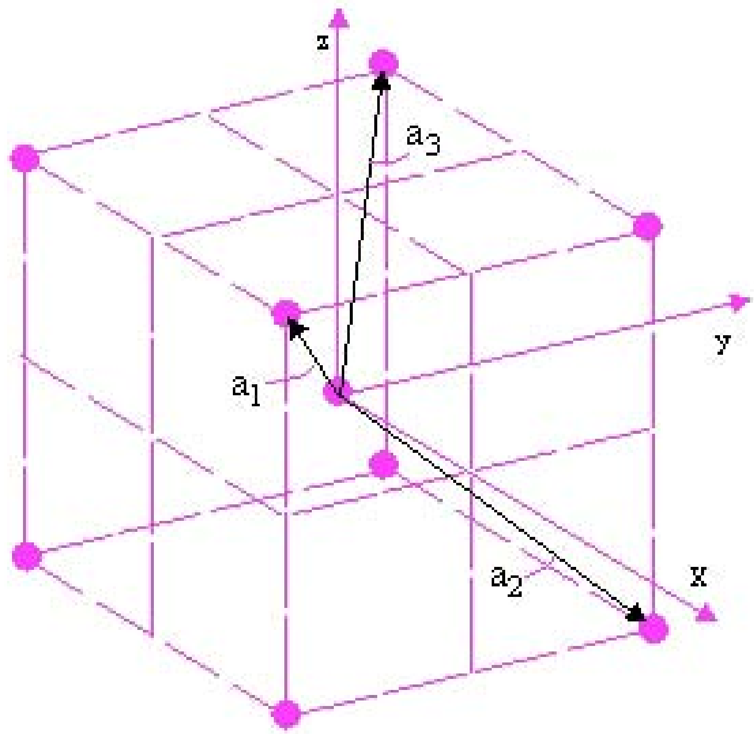
Conventional Cell
Face Centered and Body Centered



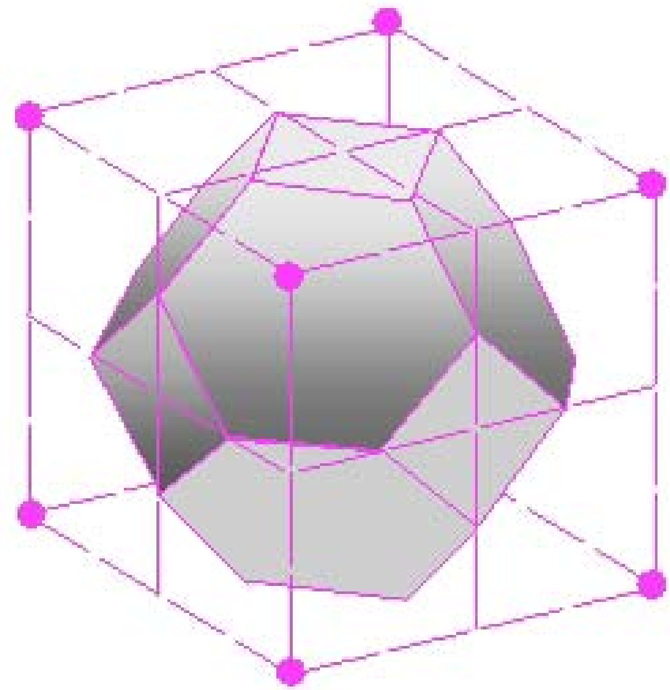
Conventional Cells
BCC: atoms at (000), (1/2,1/2,1/2)
FCC: atoms at (000), (0,1/2,1/2), (1/2,0,1/2), (1/2,1/2,0)

Ex. How many atom fractions are contained in the BCC or FCC cell?

Primitive bcc cell



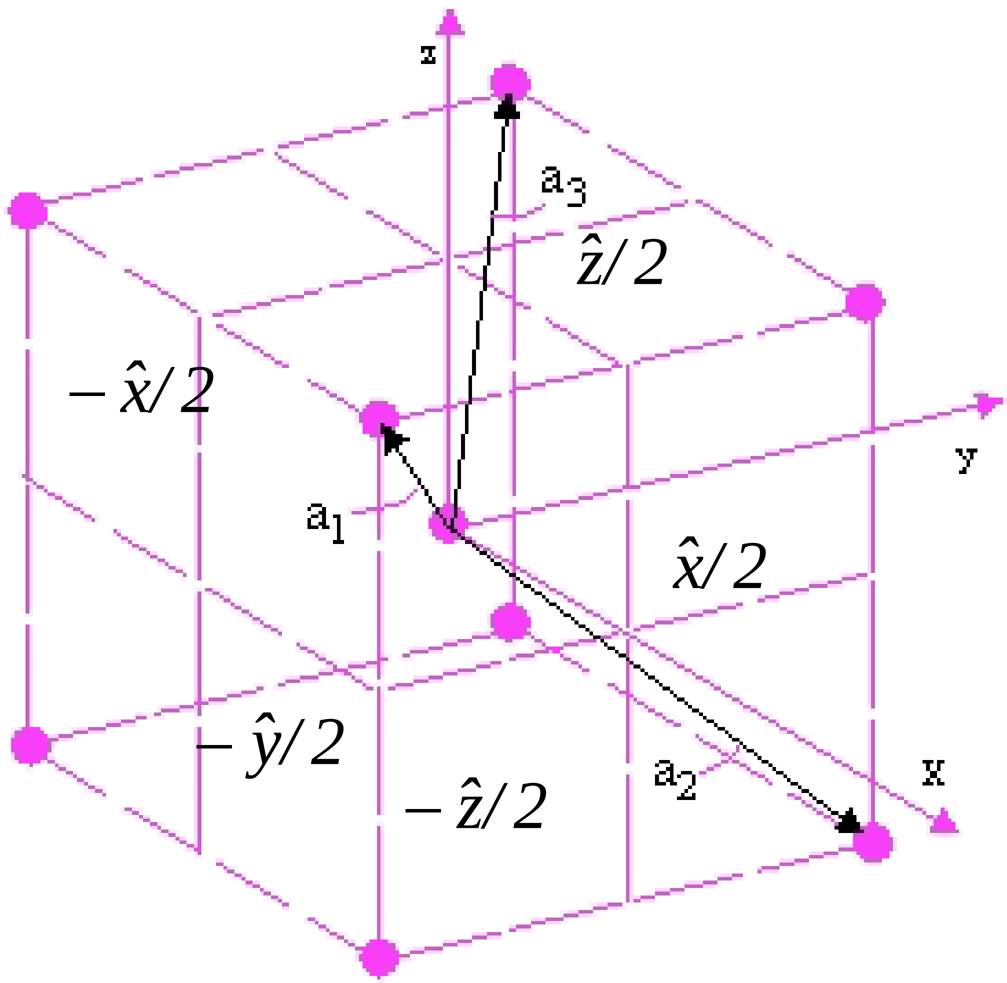
Body Centered Cubic Lattice



Wigner-Seitz Cell for
Body Centered Cubic Lattice

Regular rhombic dodecahedron

Primitive bcc cell



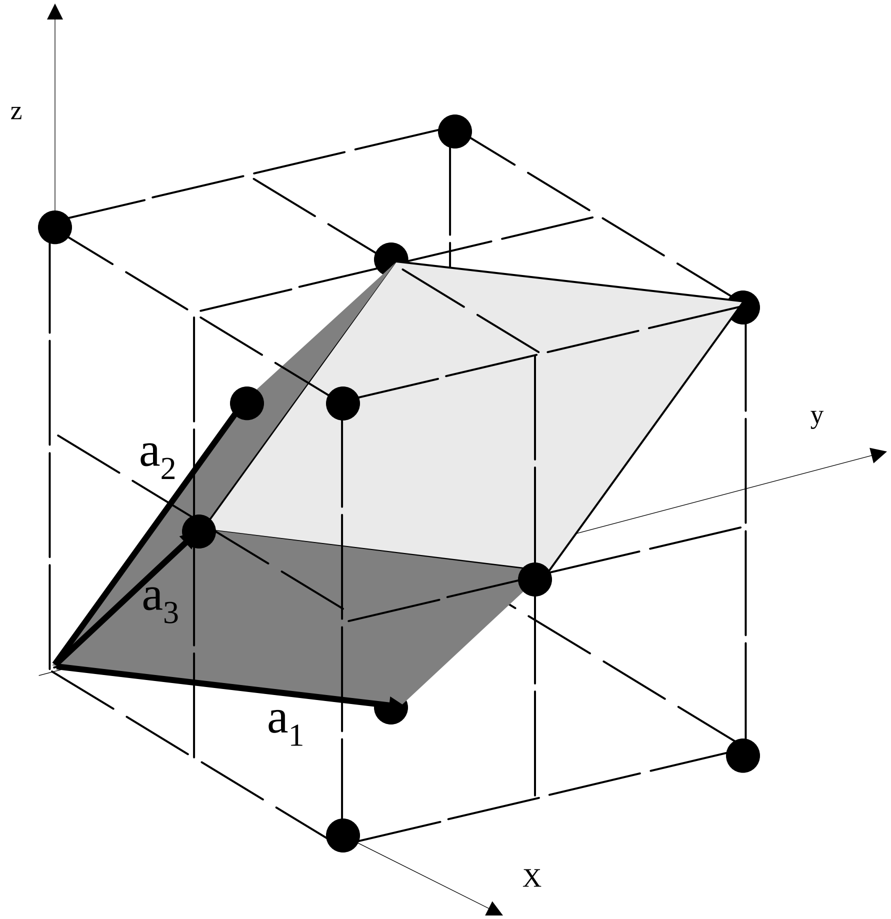
Ex. Consider a cube with unit side length.

Write down the primitive axes of the bcc cell using the unit vectors $\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}, \hat{\boldsymbol{z}}$

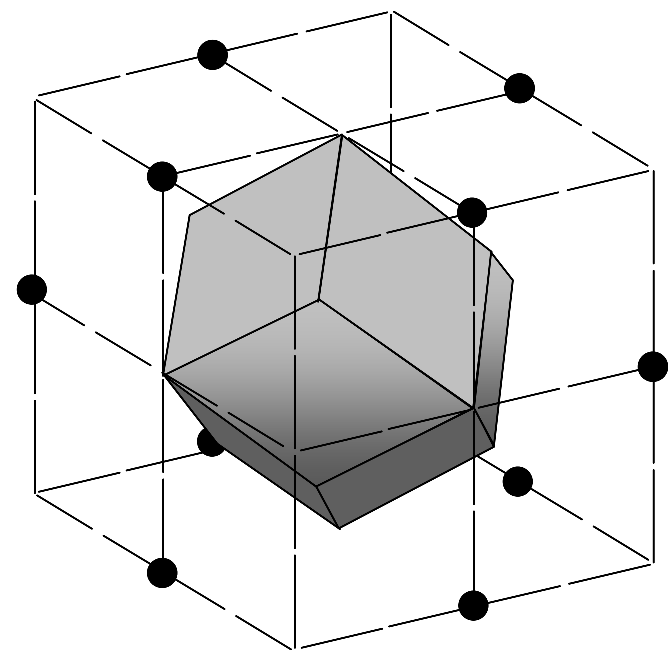
$$\boldsymbol{a_1} = \hat{x}/2 - \hat{y}/2 + \hat{z}/2$$

$$\boldsymbol{a_2} = \hat{x}/2 + \hat{y}/2 - \hat{z}/2$$

$$\boldsymbol{a_3} = \hat{x}/2 + \hat{y}/2 - \hat{z}/2$$



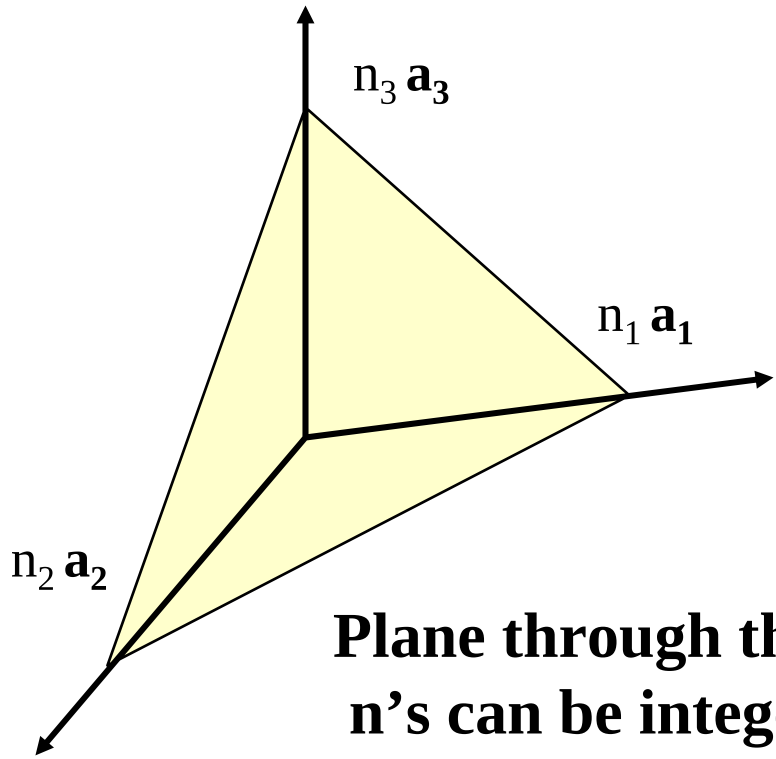
One Primitive Cell



Wigner-Seitz Cell

Face Centered Cubic Lattice

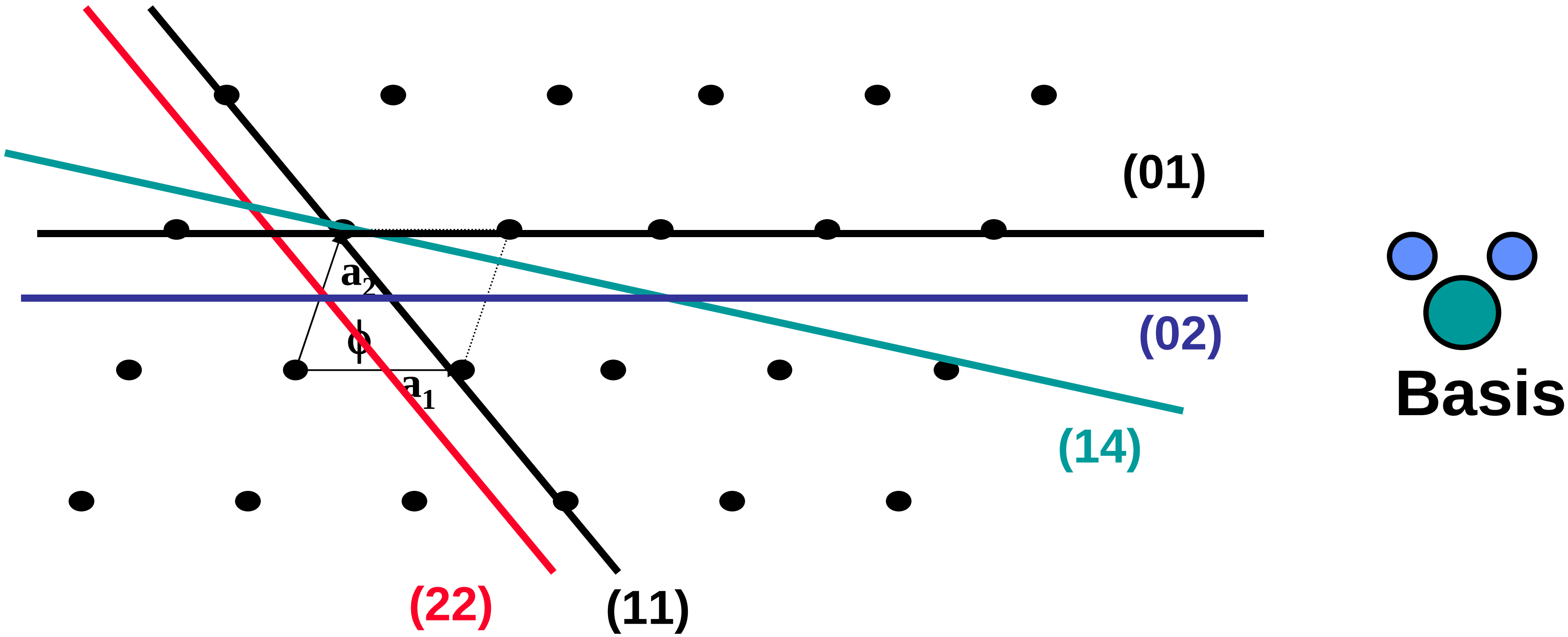
Lattice Planes - Index System



Plane through the lattice $n_1\,\mathbf{a_1}$, $n_2\,\mathbf{a_2}$, $n_3\mathbf{a_3}$
n's can be integers or rational fractions

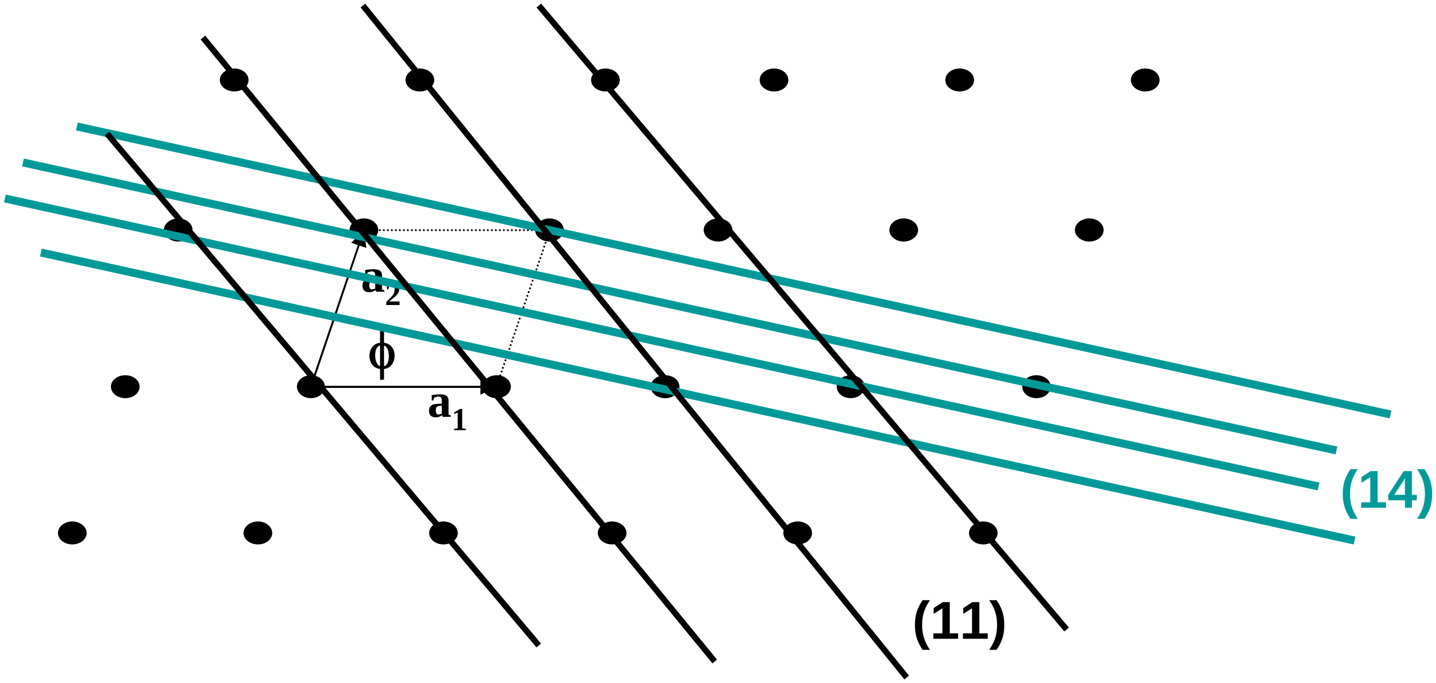
- Define the plane by the reciprocals $1/n_1$, $1/n_2$, $1/n_3$
- Reduce to three integers with same ratio h,k,l
- Plane is defined by h,k,l

Lattice planes in 2d crystals



- Infinite number of possible planes
- Can be through lattice points or between lattice points.
- The lattice planes are independent of the basis.

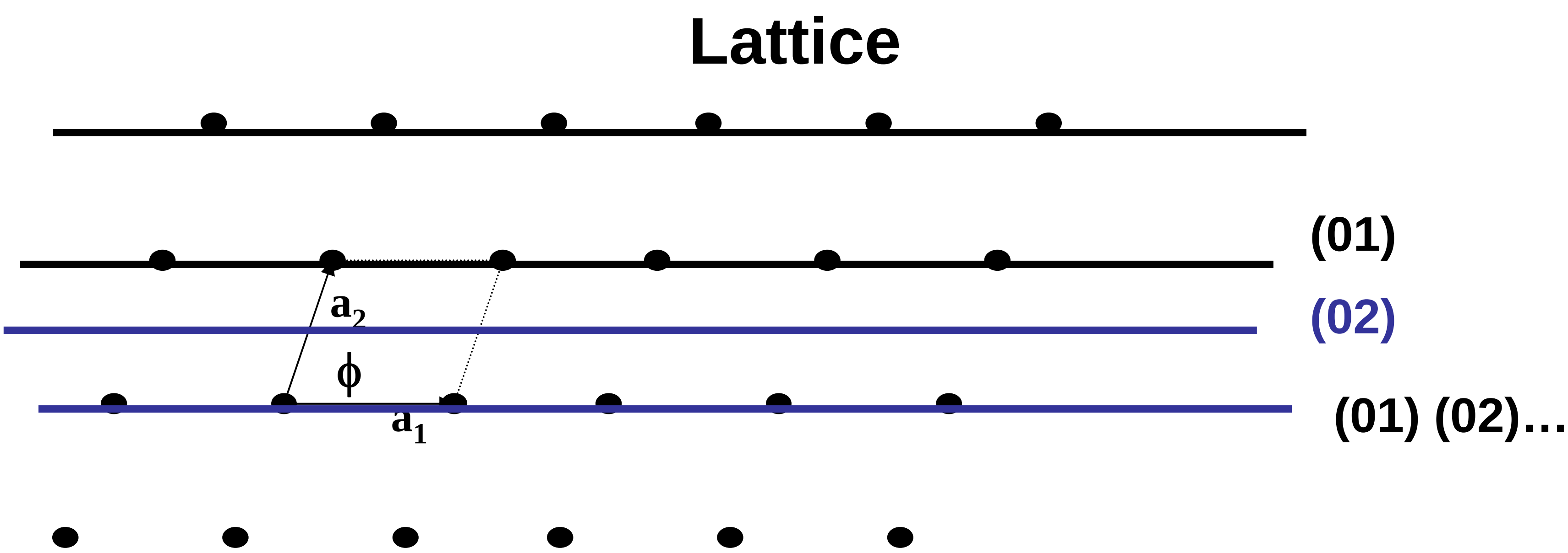
Schematic illustrations of lattice planes



- Each set of (h k) defines a family of parallel planes (e.g. planes that have the same intercept in different cells)

- Note that there always is a (h k) plane going through the origin!

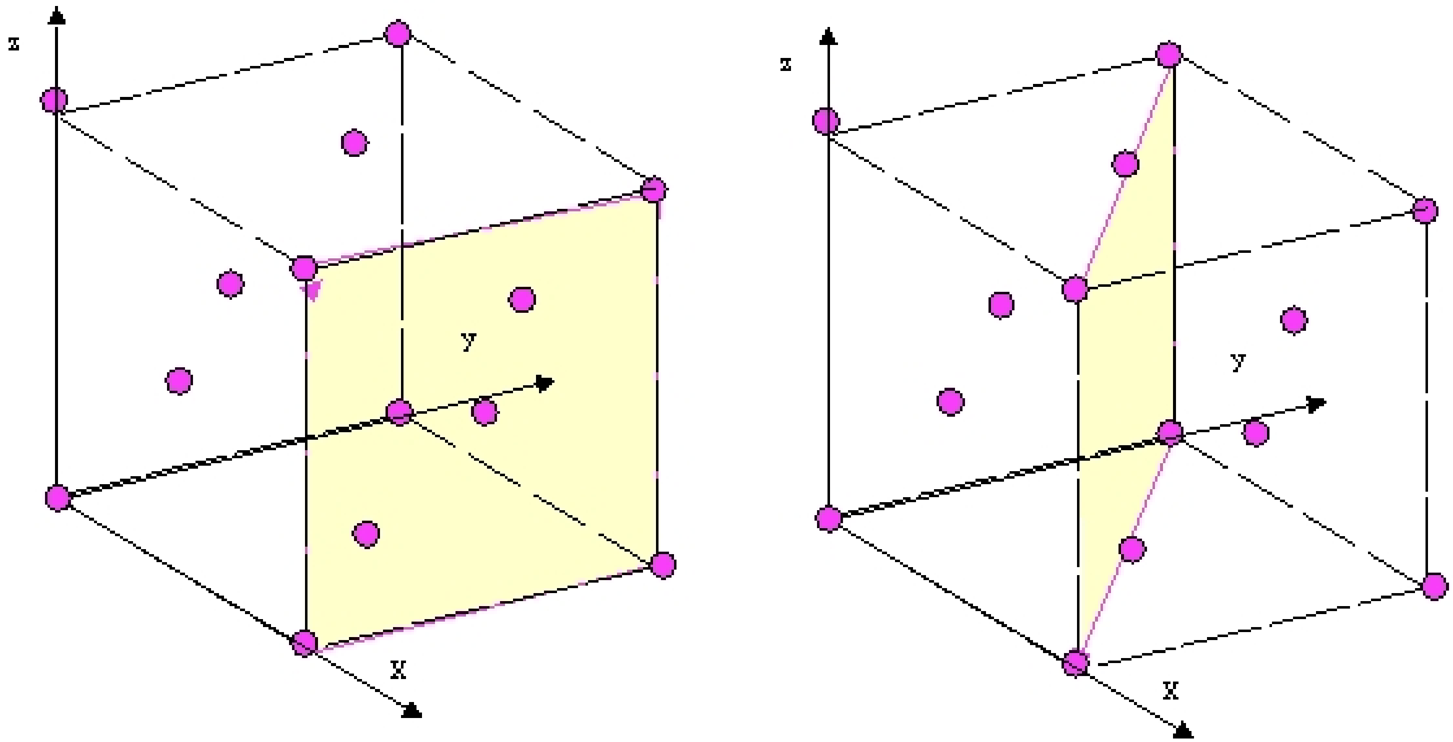
Equivalent lattice planes



- Distance between (h,k) planes: length of vector starting from cell origin and perpendicular to plane
- Low index planes: more lattice points, more widely spaced
- High index planes: less lattice points, more closely spaced

- If the Miller indices contain a common divisor **n**, only every **n**th plane contains lattice points

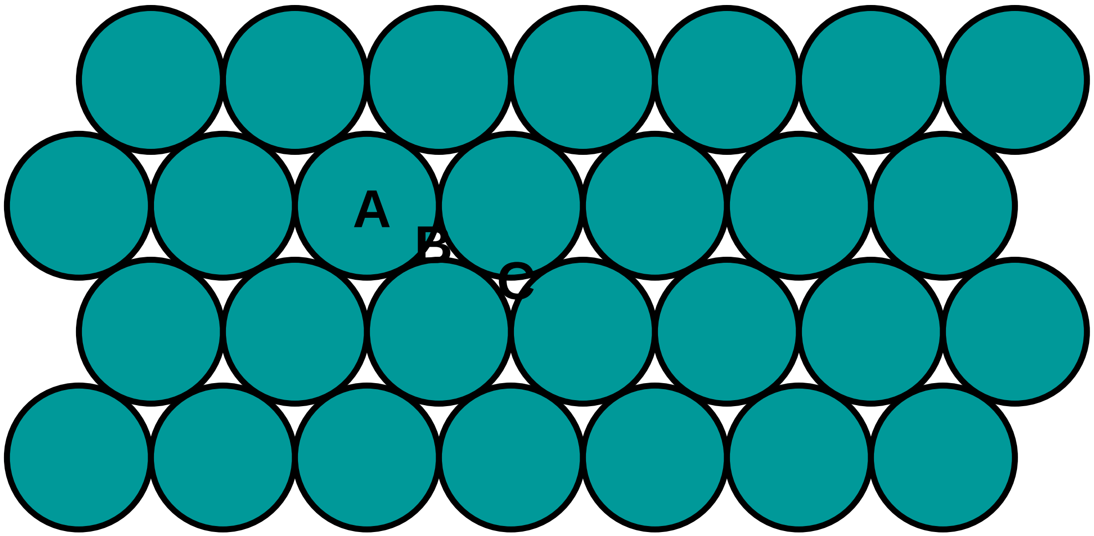
Lattice planes in cubic crystals



(100) and (110) planes in a cubic lattice
(illustrated for the fcc lattice)

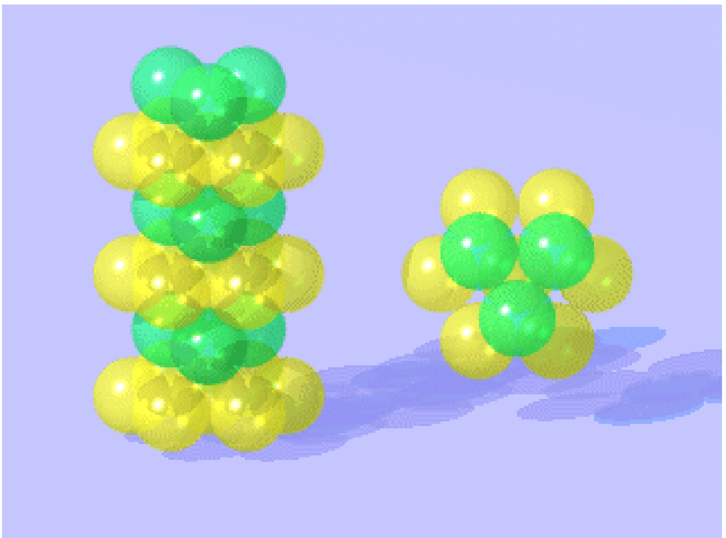
(100) plane parallel to yz plane; (110) plane parallel to z axis

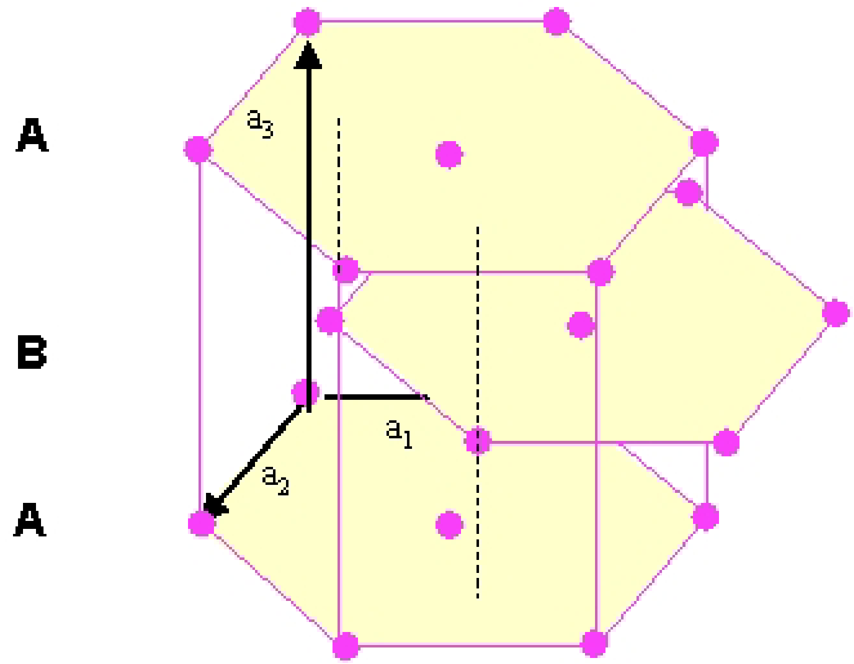
Stacking hexagonal 2d layers to make close packed 3d crystal



- Can stack each layer in one of two ways, B or C above A
- Either way, each sphere has 12 equal neighbors
- 6 in plane, 3 above, 3 below

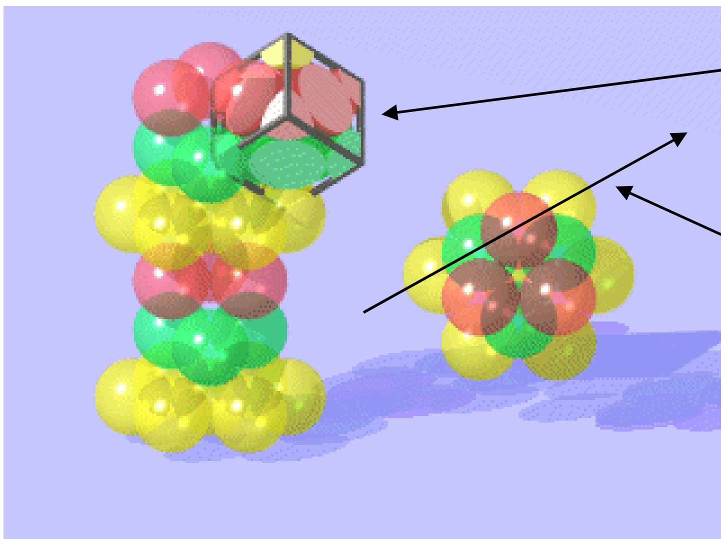
Stacking hexagonal 2d layers to make hexagonal close packed (hcp) 3d crystal





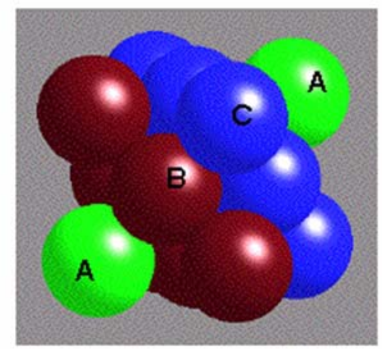
- Stacking sequence: ABABAB
- Hexagonal Bravais lattice, basis of 2 atoms

Stacking hexagonal 2d layers to make a face centered cubic (fcc) 3d crystal



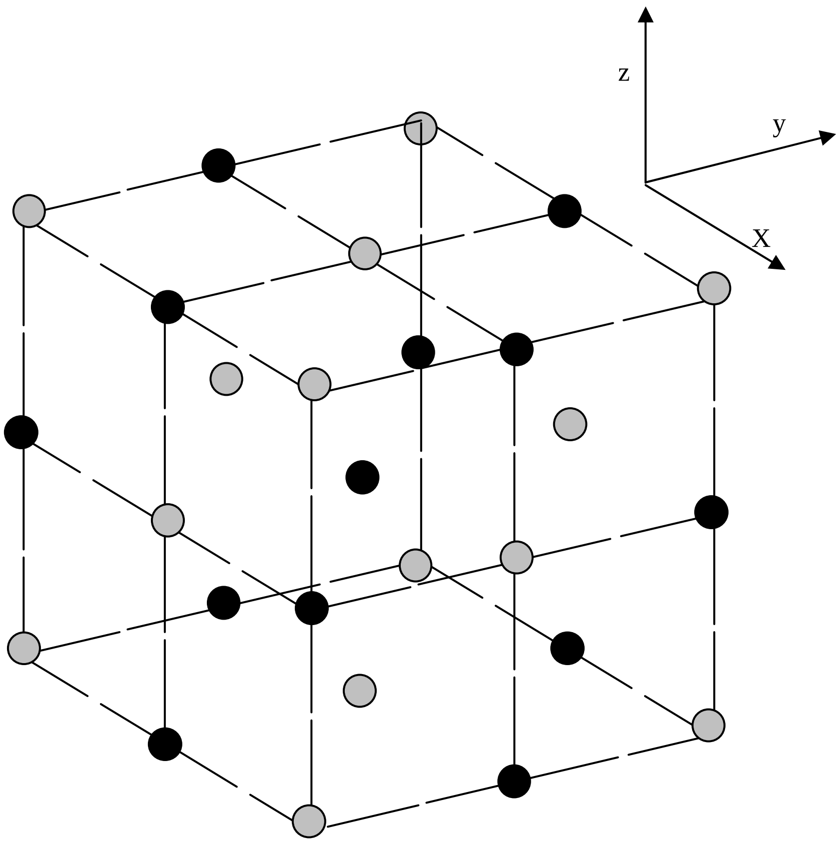
Cube

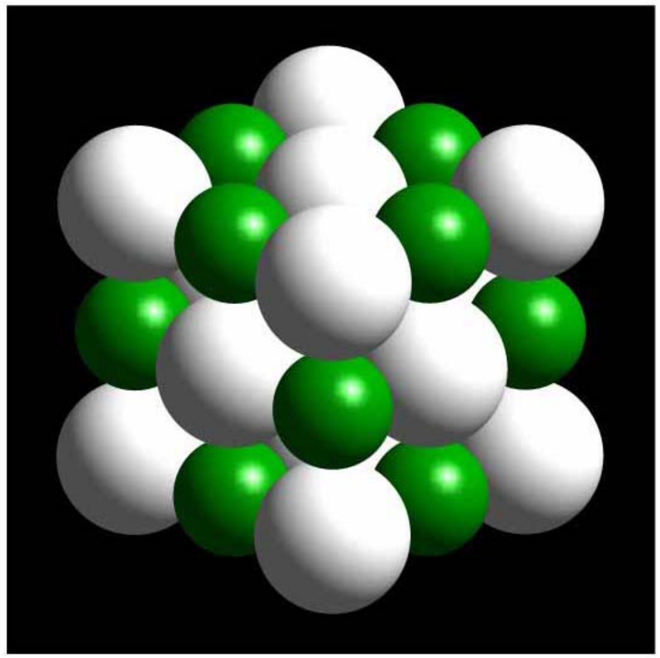
Note spheres in a line parallel to [110] direction in cube



- Stacking sequence: ABCABCABC
- Leads to an fcc lattice
- Basis of 1 atom

NaCl Structure

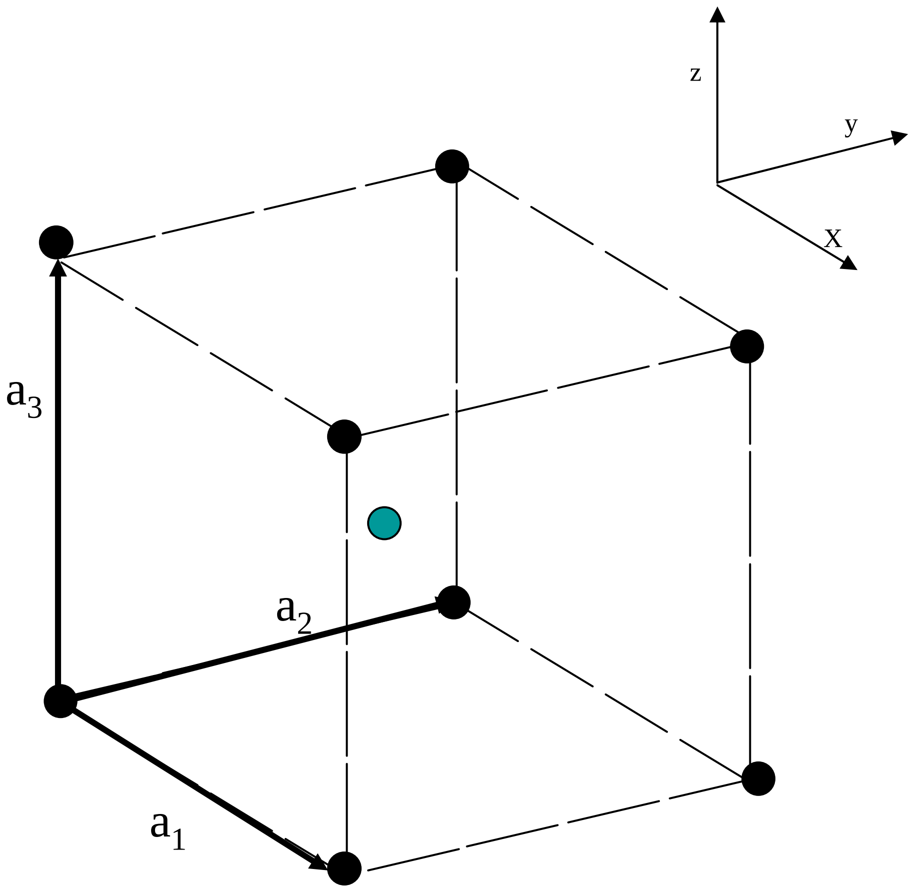




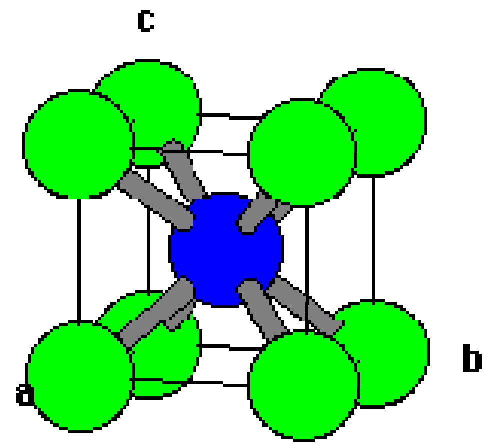
Face Centered Cubic Bravais Lattice
Two atoms (one Na, one Cl) per basis
In the conventional cubic lattice there are eight atoms per basis.

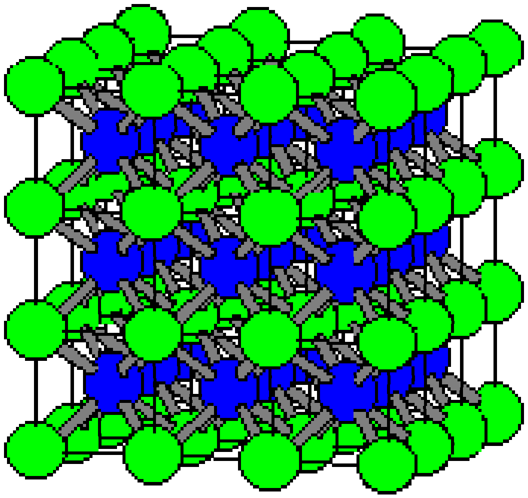
Ex. What are these eight atoms' positions?

CsCl Structure



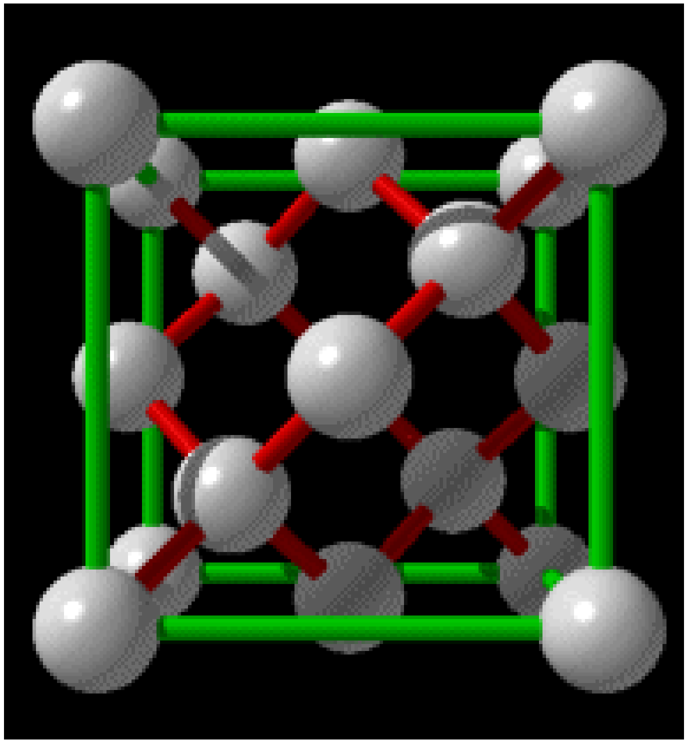
Simple Cubic Bravais Lattice
Two atoms per basis

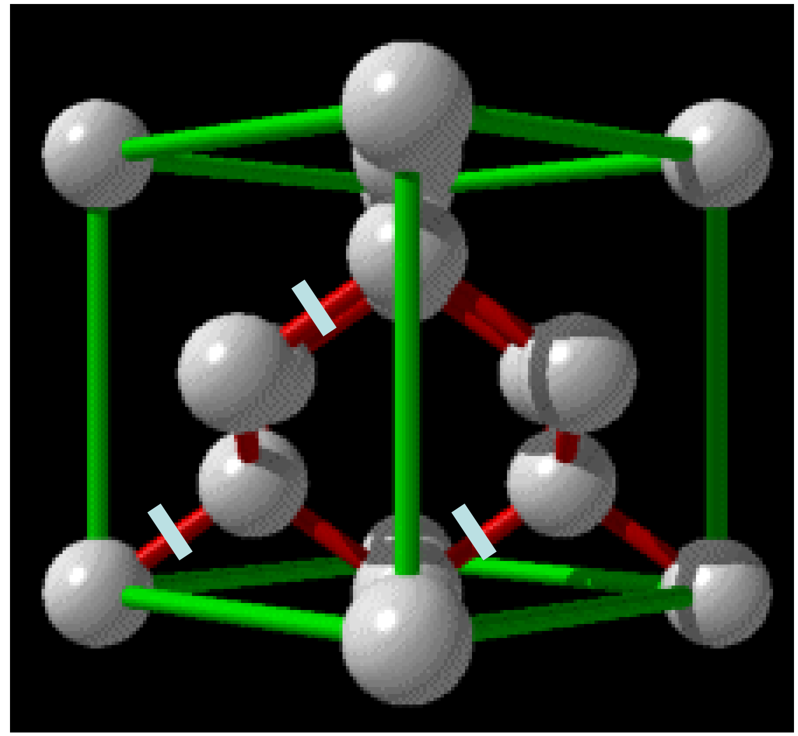




From http://www.ilpi.com/inorganic/structures/cscl/index.html

Diamond crystal structure





Face Centered Cubic Bravais Lattice
Two identical atoms per basis
Ex. What are the basis atoms' positions? How does the diamond structure differ from the NaCl structure?

Next Time

- Diffraction from crystals

- Reciprocal lattice

- Read Kittel Ch 2