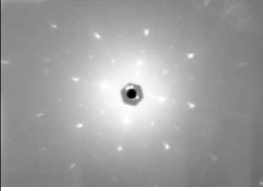



Welcome to

Phys 446: Solid State Physics / Optical Properties

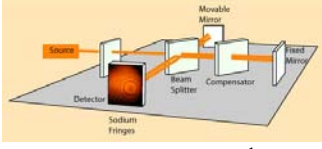


Fall 2015



Lecture 1

Andrei Sirenko, NJIT



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Instructor:

Andrei Sirenko
Professor at the Dept. of Physics, NJIT
<http://web.njit.edu/~sirenko>

468 Tiernan
Office hours: Before the classes or by appointment
973-596-5342

Class Schedule:

Monday 1 pm - 4 pm | FMH 407

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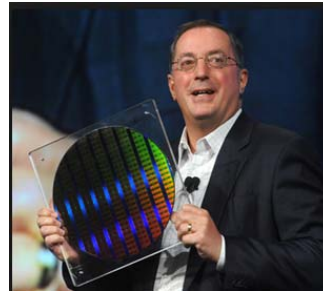
Plan for today:

- Introduction to the Course
- Crystals



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Course Elements:

Textbooks:

M. A. Omar, "Elementary Solid State Physics", Addison-Wesley, 1993.

Charles Kittel, Introduction to Solid State Physics, 8th Edition, Wiley, 2004.

Supplemental texts:

- H. Ibach, H. Lüth, "Solid-State Physics. An Introduction to Principles of Materials Science", Springer, 2003.
- J. S. Blakemore, "Solid State Physics", Third Edition, Cambridge University Press, 1985
- P. Yu and M. Cardona, "Fundamentals of semiconductors"
- N. W. Ashcroft and N. D. Mermin, "Solid State Physics"

Lecture Slides

Demonstrations in the Experimental Lab at NJIT

- Raman Scattering in Diamond
- High-Resolution X-ray Diffraction in Silicon wafer
- Transmission in InP-based multilayer device structure
- Micro-beam Photoluminescence in InGaAsP-based waveguide device structure

Grade Components:

- Homework: 10 %
- Research project: 10 %
- Two in-class exams: 15% each;
- Final exam: 50%

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Course Goals:

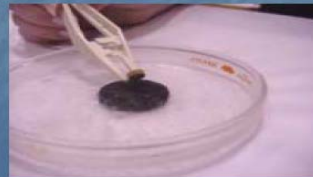
This course integrates theory of Solid State Physics with experimental demonstrations in the Research Physics Lab. The course will provide a valuable theoretical introduction and an overview of the fundamental applications of the physics of solids. This course includes theoretical description of crystal and electronic structure, lattice dynamics, and optical properties of different materials (metals, semiconductors, dielectrics, magnetic materials and superconductors), based on the classical and quantum physics principles. Several advanced experiments of X-ray diffraction, Raman Scattering, Photoluminescence, *etc.*, will be carried out in the Research Physics Lab followed by their theoretical discussion.

To help you with your research projects and future jobs

Solid State Physics

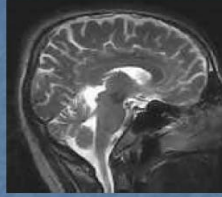
- Why study condensed matter?
- Condensed matter physics mostly concerns the study of solids, but it has been extended to amorphous substances, glasses, and liquids
 - The largest branch of modern physics
- Most of the research is done on solids, be it in crystalline or ceramic (multicrystalline powder) form

A high-temperature superconductor, cooled in liquid nitrogen, expels local magnetic fields (called the Meissner effect), and causes this magnet to levitate above it

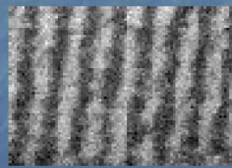
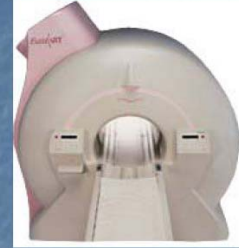


Why study solids?

- Technological spin-offs: superconductivity (MRI machines, cheap power transportation, etc), magnetic recording media, rechargeable batteries
 - New Physics!!
- What happens when we have a large no. of particles (degrees of freedom)?
- Eg. Temperature makes no sense when applied to one molecule – it must be applied to a collection of particles (eg. A gas, liquid, or solid)
- How do 10^{23} no. of particles give rise to macroscopic properties?



MRI scanners use superconductor technology



Test bits on a hard drive



Rechargeable batteries

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Outline of the course:

- I. Crystal structure, symmetry and types of chemical bonds. (Chapter 1)
 - The crystal lattice
 - Point symmetry
 - The 32-crystal classes
 - Types of bonding (covalent, ionic, metallic bonding; hydrogen and van der Waals).
- II. Diffraction from periodic structures (Chapter 2)
 - Reciprocal lattice; Brillouin zones
 - Laue condition and Bragg law
 - Structure factor; defects
 - Methods of structure analysis
 - *HKXRD. Experimental demonstration in the Physics Lab using Bruker D8 Discover XRD*
- III. Lattice vibrations and thermal properties (Chapter 3)
 - Elastic properties of crystals; elastic waves
 - Models of lattice vibrations
 - Phonons
 - Theories of phonon specific heat; thermal conduction.
 - Anharmonicity; thermal expansion
 - *Raman Scattering by phonons. Experimental demonstration in the Physics Lab using Ar-laser/SPEX 500M, CCD-based Raman Scattering setup*
- IV. Electrons in metals (Chapters 4-5)
 - Free electron theory of metals
 - Fermi Statistics
 - Band theory of solids
- V. Semiconductors (Chapters 6-7)
 - Band structure.
 - Electron statistics; carrier concentration and transport; conductivity; mobility
 - Impurities and defects
 - Magnetic field effects: cyclotron resonance and Hall effect
 - Optical properties; absorption, photoconductivity and luminescence
 - Basic semiconductor devices
 - *Photoluminescence. Experimental demonstration in the Physics Lab using Nd:YAG laser/SPEX-based Photoluminescence setup*
- VI. Dielectric properties of solids (Chapters 8)
 - Dielectric constant and polarizability (susceptibility)
 - Dipolar polarizability, ionic and electronic polarizability
 - Piezoelectricity; pyro- and ferroelectricity
 - Light propagation in solids
- VII. Magnetism (Chapters 9)
 - Magnetic susceptibility
 - Classification of materials; diamagnetism, paramagnetism
 - Ferromagnetism and antiferromagnetism
 - Magnetic resonance
 - Multiferroic Materials
- VIII. Superconductivity (Chapter 10)

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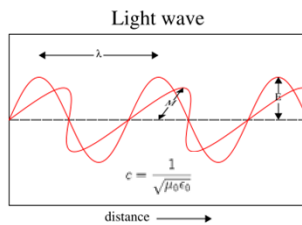
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Lectures:

- Presentation of the concepts and techniques of SSP.
- Demonstrations.
- HW discussions
- Lectures are not a substitute for reading the textbook and independent literature search
Read ahead; you'll get more from lecture.
- Slides are posted on the course web. Slides will be updated during the Semester
Use these as a study guide/note taking aid

Scope and Requirements

$$\begin{aligned}\nabla \cdot \mathbf{E} &= 0 \\ \nabla \times \mathbf{E} &= -\frac{\partial \mathbf{B}}{\partial t} \\ \nabla \cdot \mathbf{B} &= 0 \\ \nabla \times \mathbf{B} &= \mu_0 \epsilon_0 \frac{\partial \mathbf{E}}{\partial t}\end{aligned}$$



λ = wave length
 E = amplitude of electric field
 M = amplitude of magnetic field

Required for Phys-446

$$c = 299792458 \text{ m / s,}$$

PHYS-III and PHYS 432 and 433 (E&M-I and II)

Familiarity with basic principles of quantum mechanics (Schrödinger equation, wave function, energy levels, spin)

Knowledge of basics of statistical physics (classical statistics, Bose-Einstein and Fermi-Dirac statistics)

Homework

- Assignments (~6 in total) will be due weekly, usually on Mondays. Assignments are due at the beginning of class.
- Homework problems, lectures, and text readings will form the basis of the exam problems.

Project

Students will perform a research project on a selected topic of contemporary solid state physics (of their choice) by reviewing scientific journal articles focusing on the effect chosen. A formal oral presentation (~10 slides) will be required.

Exams:

There will be two in-class exams and a final exam.

- Allowed to use **lecture notes** and formula sheets (but no books, no internet, no phone calls).
- Not allowed to discuss the problems with other students.

Academic honesty

Students are encouraged to:

- discuss the lectures and textbook material
- work together on homework problems
- study together for exams

But not allowed to:

- present other people's work as your own (including copying another student's homework as well as using of problem solutions found in the Internet or elsewhere)
- discuss problems or questions during exams



Today: crystal structures

Lecture 1-1

“...What do you know about crystals ?
“They make nice chandeliers !?..”

Superman Returns



Lecture 1



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- The habit of a crystal describes its overall shape
- These offer clues to how the atoms are arranged
- But, the growth (and shape) of crystals is also determined by a number of factors, including:
 - (1) Temperature
 - (2) Pressure
 - (3) pH (acid or basic environment), etc
- So, scientists need another way to see how crystals form – the first way to do this is by x-ray diffraction (we will discuss this more in Chapter 2)
- Why do x-rays tell us about how the atoms are arranged?

Hexagonal beryl



Monoclinic gypsum



Trigonal quartz



Amorphous amber
(no underlying crystal symmetry)

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Experimental techniques to measure solids

- Scattering: x-rays, neutrons, electrons (information about where the atoms are, excitations)
- Resonance methods: nuclear magnetic resonance, muon spin resonance (magnetism)
- Thermodynamic properties: specific heat, thermal conductivity (what is carrying the heat?)
- Electronic properties: resistivity, Hall effect, photoemission (how do the electrons move? Metal, semiconductor, or insulator?)
- Optical measurements : microwave, infrared, etc. (how does EM radiation interact with the electrons? What can this tell us?)

Heat capacity (low temperatures)



Muon spin resonance (at TRIUMF)



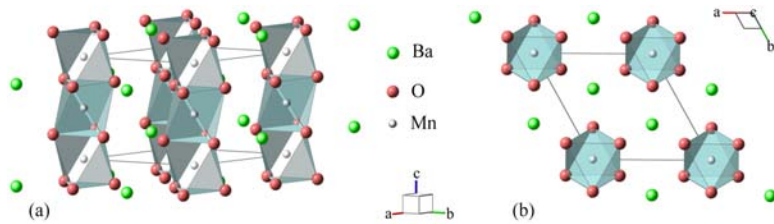
Neutron scattering (at NIST, USA)

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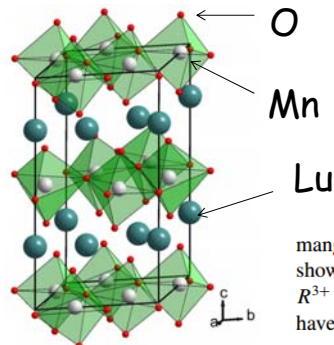
15

Examples: BaMnO₃ and LuMnO₃ crystals



Crystallographic structure of 2H-BMO featuring face-sharing MnO₆ octahedrons

(space group $P6_3mc$) from (a) side view and (b) top view.



Crystal structure of hexagonal rare-earth manganites $RMnO_3$ in the ferroelectric phase. View is along (110) showing two layers of MnO₅ trigonal bipyramids and two layers of R^{3+} ions. HoMnO₃ lattice parameters and internal atomic coordinates have been used.

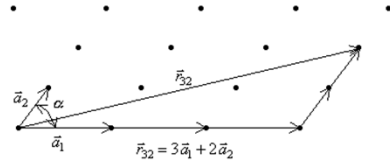
Today: crystal structures (Omar Ch. 1.1.-1.6.)

Crystal: atoms are arranged so that their positions are periodic in all three dimensions

Atoms are bound to one another → well defined equilibrium separations;

many identical atoms → minimum energy requires every identical atom to be in

identical environment → 3D periodicity



$$\vec{r}_n = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$$

Ideal crystal: perfect periodicity

Real crystals are never perfect:

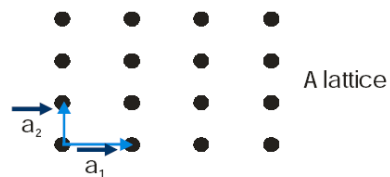
- surface
- impurities and defects
- thermal motion of atoms (lattice vibrations)

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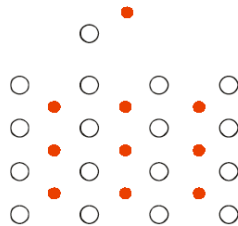
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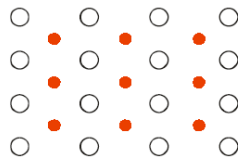
Crystal structure = lattice + basis



A basis



A crystal structure



We need to identify the symmetry (lattice vectors) and the lattice contents (basis) to fully describe a structure.

(1) How do we choose lattice vectors? (This will lead us to thinking about unit cells)

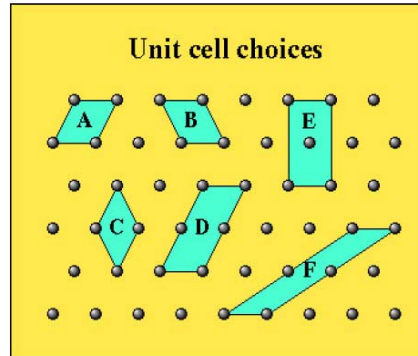
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Choice of primitive cells

- Which unit cell is a good choice?
- A, B, and C are primitive unit cells. Why?
- D, E, and F are not. Why?
- Notice: the volumes of A, B, and C are the same. Also, the choice of origin is different, but it doesn't matter
- Also: There is only one lattice point in the primitive unit cells.



Definitions

The periodic array of points is called crystal lattice.

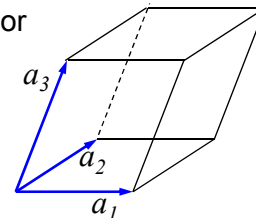
For every lattice point there is a group of atoms (or single atom) called *basis* of the lattice

Don't confuse with a_1, a_2, a_3 - *basis vectors*
 parallelogram formed by the basis vectors –
unit cell

if a unit cell contains only one lattice point, it is
 called a *primitive cell* (minimum volume)

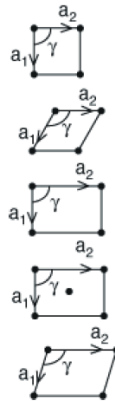
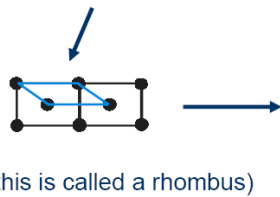
Bravais lattices – all lattice points
 are equivalent

2D case – 5 Bravais lattices in the next slide



The 2D Bravais lattices

Note that this is the proper primitive cell for the centered rectangular lattice type (why? It contains only one lattice point)



square	$a_1 = a_2$	$\gamma = 90^\circ$
hexagonal	$a_1 = a_2$	$\gamma = 120^\circ$
rectangular	$a_1 \neq a_2$	$\gamma = 90^\circ$
centered rectangular	$a_1 \neq a_2$	$\gamma = 90^\circ$
oblique	$a_1 \neq a_2$	$\gamma \neq 90^\circ, 120^\circ$

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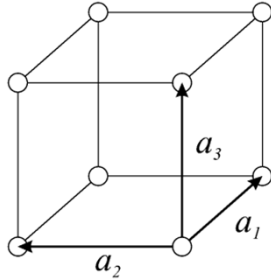
7 crystal systems and 14 Bravais lattices in 3D

<p>triclinic $a \neq b \neq c$ $\alpha, \beta, \gamma \neq 90^\circ$</p>	<p>monoclinic $a \neq b \neq c$</p> <p>P $\alpha \neq 90^\circ$ $\beta, \gamma = 90^\circ$</p> <p>C $\alpha \neq 90^\circ$ $\beta, \gamma = 90^\circ$</p>	<p>orthorhombic $a \neq b \neq c, \alpha = \beta = \gamma = 90^\circ$</p> <p>P C I F</p>	
<p>tetragonal $a = b \neq c, \alpha = \beta = \gamma = 90^\circ$</p> <p>P I</p>	<p>rhombohedral (trigonal) $a = b = c, \alpha = \beta = \gamma \neq 90^\circ$</p>	<p>cubic $a = b = c, \alpha = \beta = \gamma = 90^\circ$</p> <p>P I F</p>	<p>hexagonal $a = b \neq c, \alpha = \beta = 90^\circ, \gamma = 120^\circ$</p>

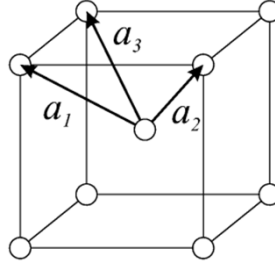
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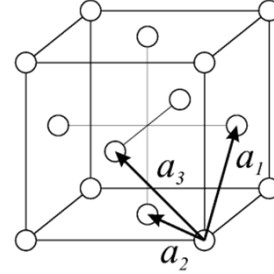
Cubic lattices: SC, BCC and FCC



simple cubic



bcc
*Body-centered
cubic*



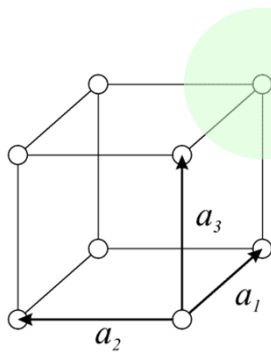
fcc
Face-centered cubic

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Cubic lattices: SC



simple cubic

Packing fraction = $\frac{(4/3)\pi(a/2)^3}{(a^3)}$
(atomic volume) / (bravais unit cell volume)

$= \pi / 6$

- The simple cubic has 1 lattice point per unit cell, with a total area of a^3
- Number of nearest neighbours: 6
- Nearest neighbour distance: a
- Number of next-nearest neighbours: 12
- Next-nearest neighbour distance: $\sqrt{2}a$ (prove this!)

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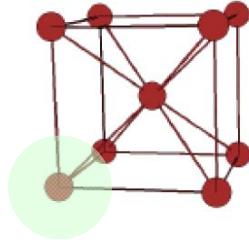
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The Body-Centred Cubic Lattice

(Li (at room temp.), Na, K, V, Cr, Fe, Rb, Nb, Mo, Cs, Ba, Eu, Ta)

Body-Centred Cubic Lattice (BCC)



$$\text{Packing fraction} = \frac{\text{(atomic volume)}}{\text{(bravais unit cell volume)}} = \frac{(4/3)\pi(\sqrt{3}a/4)^3}{(a^3/2)} = \sqrt{3}\pi / 8$$

- The body-centred cubic lattice has 2 lattice points per unit cell, with a total primitive cell volume of $a^3/2$
- Number of nearest neighbours: 8
- Nearest neighbour distance: $\sqrt{3} a/2 = 0.866 a$ (prove this!)
- Number of next-nearest neighbours: 6 (where are these?)
- Next-nearest neighbour distance: a (prove this!)

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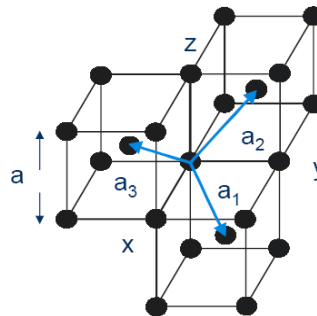
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The Body-Centred Cubic Lattice

- The primitive cell of the BCC lattice is defined by the translation vectors:

$$\begin{aligned} \vec{a}_1 &= \frac{1}{2} a (\vec{x} + \vec{y} - \vec{z}) \\ \vec{a}_2 &= \frac{1}{2} a (-\vec{x} + \vec{y} + \vec{z}) \\ \vec{a}_3 &= \frac{1}{2} a (\vec{x} - \vec{y} + \vec{z}) \end{aligned}$$

where \vec{x} , \vec{y} , and \vec{z} are the Cartesian unit vectors. These translation vectors connect the lattice pt at the origin to the points at the body centres (and make a rhombohedron)



See figure 11 in Kittel for a picture of the primitive cell in more detail

The angle between

\vec{a}_1 and \vec{a}_2 vectors?

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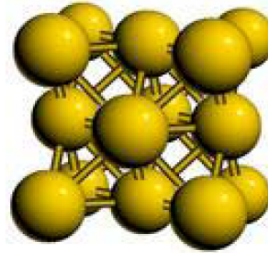
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The Face-Centred Cubic Lattice

(Al, Cu, Ni, Sr, Rh, Pd, Ag, Ce, Tb, Ir, Pt, Au, Pb, Th)

- The face-centred cubic lattice has 4 lattice points per unit cell, with a total primitive cell volume of $a^3/4$
- Number of nearest neighbours: 12
- Nearest neighbour distance: $a/\sqrt{2} = 0.707 a$ (prove this!)
- Number of next-nearest neighbours: 6 (where are these?)
- Next-nearest neighbour distance: a (prove this!)



Packing fraction =
(atomic volume)/
(bravais unit cell
volume)

$$= \sqrt{2}\pi / 6$$

(do this on
your own)

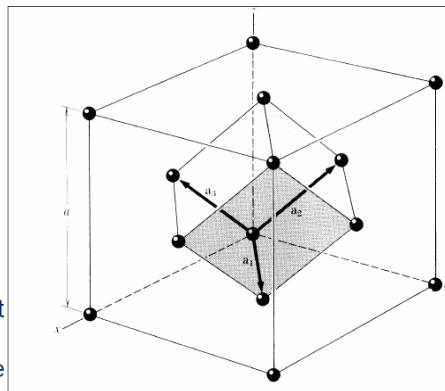
The Face-Centred Cubic Lattice

- The primitive cell of the FCC lattice is defined by the translation vectors:

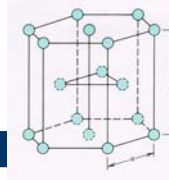
$$\begin{aligned} \vec{a}_1 &= \frac{1}{2} a (\vec{x} + \vec{y}) \\ \vec{a}_2 &= \frac{1}{2} a (\vec{y} + \vec{z}) \\ \vec{a}_3 &= \frac{1}{2} a (\vec{z} + \vec{x}) \end{aligned}$$

where \vec{x} , \vec{y} , and \vec{z} are the Cartesian unit vectors. These translation vectors connect the lattice pt at the origin to the points at the face centres.

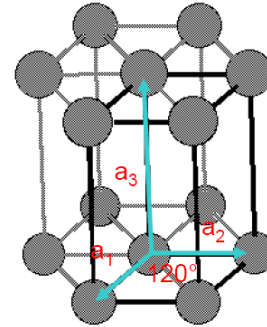
The angles between the axes are 60°



Hexagonal unit cell



- The primitive cell in a hexagonal system is a right prism based on a rhombus with an included angle of 120°
- Note here that $a_1 = a_2 \neq a_3$
- Later, we will look at the hexagonal close-packed structure, which is this structure with a basis (and is related to the fcc structure).



(primitive cell is in bold)

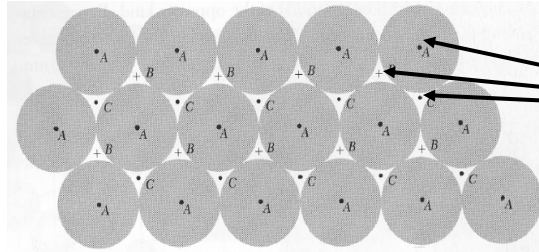
Closed-packed structures



(or, what does stacking fruit have to do with solid state physics?)

Closed-packed structures

- There are an infinite number of ways to organize spheres to maximize the packing fraction.



The centers of spheres at A, B, and C positions (from Kittel)

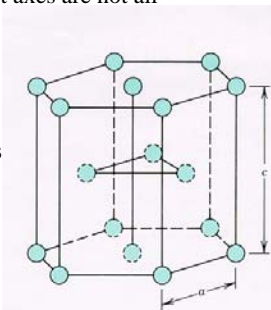
There are different ways you can pack spheres together. This shows two ways, one by putting the spheres in an ABAB... arrangement, the other with ACAC.... (or any combination of the two works)

(3) The Hexagonal Closed-packed (HCP) structure

Be, Sc, Te, Co, Zn, Y, Zr, Tc, Ru, Gd, Tb, Py, Ho, Er, Tm, Lu, Hf, Re, Os, Tl

- The HCP structure is made up of stacking spheres in a ABABAB... configuration
- The HCP structure has the primitive cell of the hexagonal lattice, with a basis of two identical atoms
- Atom positions: $000, \frac{2}{3} \frac{1}{3} \frac{1}{2}$ (remember, the unit axes are not all perpendicular)
- The number of nearest-neighbours is 12
- The ideal ratio of c/a for this packing is $(\frac{8}{3})^{1/2} = 1.633$

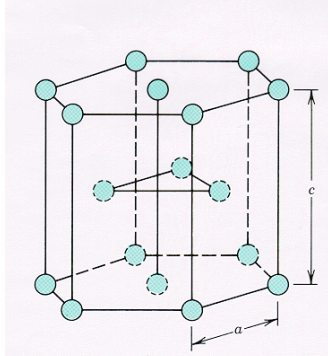
Rotated three times



Conventional HCP unit cell

HCP structure and Golden Ratio

- The ideal ratio of c/a for this packing is $(8/3)^{1/2} = 1.633$



Conventional HCP unit cell

Lecture 1

Phi ($\Phi = 1.618033988749895\dots$)

It can be derived with a number of **geometric constructions**, each of which divides a line segment at the unique point where:

the ratio of the whole line (A) to the large segment (B)
is the same as
the ratio of the large segment (B) to the small segment (C).

In other words, A is to B as B is to C.

This occurs only where A is 1.618 ... times B **and** B is 1.618 ... times C.

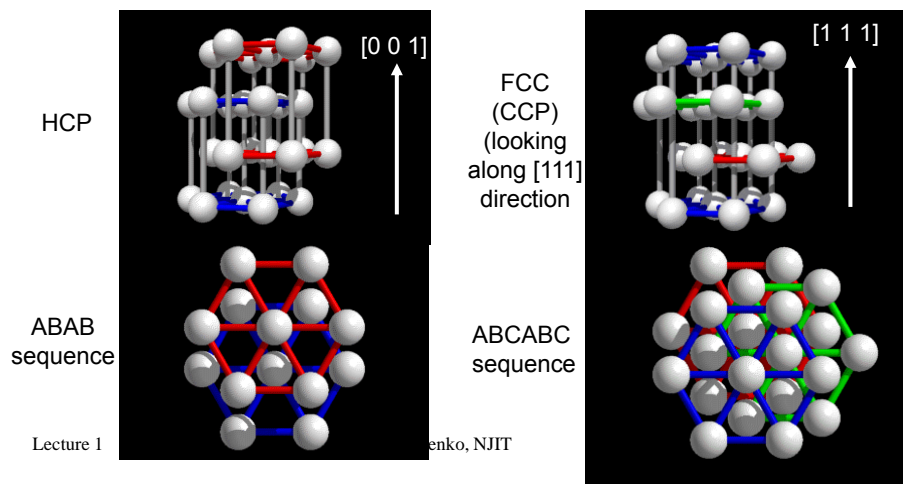
This ratio has been used by mankind for centuries

Its use may have started as early as with the Egyptians in the design of the pyramids,

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The FCC and hexagonal closed-packed structures (HCP) are formed from packing in different ways. FCC (sometimes called the cubic closed-packed structure, or CCP) has the stacking arrangement of ABCABCABC... HCP has the arrangement ABABAB....



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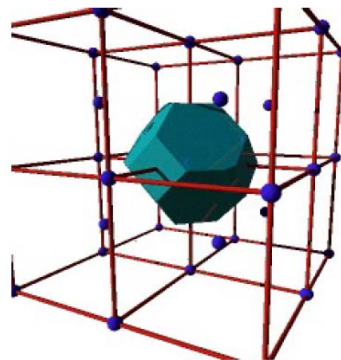
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HCP and FCC structures

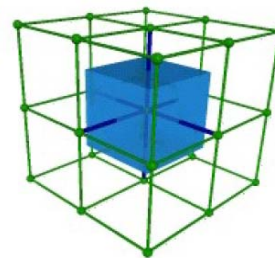
- The hexagonal-closed packed (HCP) and FCC structures both have the ideal packing fraction of 0.74 (Kepler figured this out hundreds of years ago)
- The ideal ratio of c/a for this packing is $(8/3)^{1/2} = 1.633$ (see Problem 3 in Kittel)
- Why aren't these values perfect for real materials?
- Why would real materials pick HCP or FCC (what does it matter if they pack the same?)

Crystal	c/a
He	1.633
Be	1.581
Mg	1.623
Ti	1.586
Zn	1.861
Cd	1.886
Co	1.622
Y	1.570
Zr	1.594
Gd	1.592
Lu	1.586

Wigner-Seitz cells



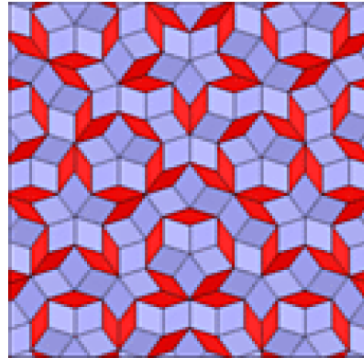
BCC lattice



Simple cubic lattice

Fivefold rotations and quasicrystals

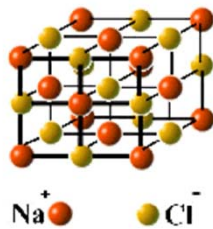
- It turns out that mathematicians discovered that you can only fill space by using rotations of unit cells by 2π , $2\pi/2$, $2\pi/3$, $2\pi/4$, and $2\pi/6$ radians (or, by 360° , 180° , 120° , 90° , and 60°)
- But, rotations of the kind $2\pi/5$ or $2\pi/7$ do not fill space!
- A quasicrystal is a quasiperiodic nonrandom assembly of two types of figures (since we need two types, it is not a Bravais lattice – you cannot fill space with just one repeating unit cell)
- We will discuss these in Chapter Two



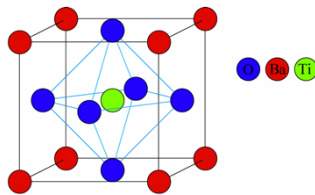
Penrose tiling in 2D

Examples

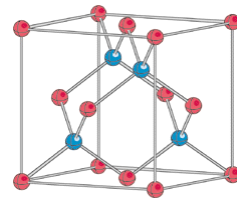
rock salt



perovskite (e.g. BaTiO_3)



diamond (Si, Ge)
zincblende (GaAs ...)



What are the Bravais lattices for these structures?
How many atoms are in the basis, and what are their positions?

fcc

O_h

cubic

fcc

T_d

Elements of symmetry

In addition to periodicity (translation) each lattice can have other symmetry properties:

- Inversion center I
- Reflection (mirror) plane
- Rotation axes. Only 2-, 3-, 4-, and 6-fold rotations are compatible with translation invariance
- Rotation-inversion axes

Point symmetry

Every crystal lattice may be described by a particular combination of symmetry operations determined by symmetry of the basis and the symmetry of the Bravais lattice.

There are **32 crystal classes (point groups)**

Combining with translational symmetries, one obtains 230 **space groups**

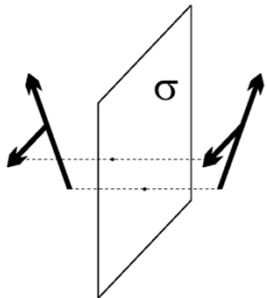
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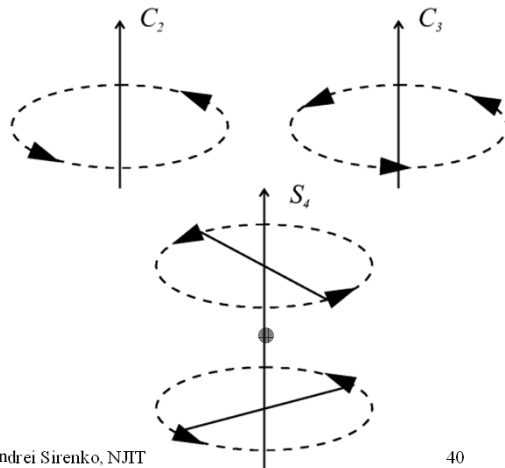
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Elements of symmetry

- Inversion center I
- Reflection (mirror) plane
- Rotation axes. Only 2-, 3-, 4-, and 6-fold rotations are compatible with translation invariance
- Rotation-inversion axes



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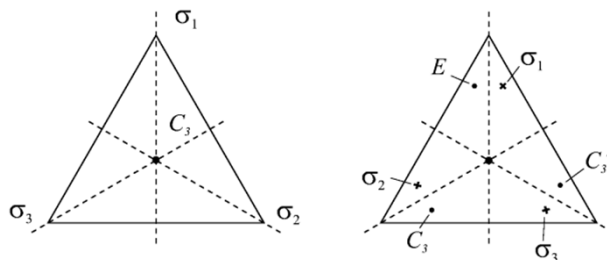


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Symmetry group example: C_{3v}

- Inversion center I
- Reflection planes: 3
- Rotation axes. Only 3- fold rotation



$C_3, C_3^2, \sigma_1, \sigma_2, \sigma_3, E.$

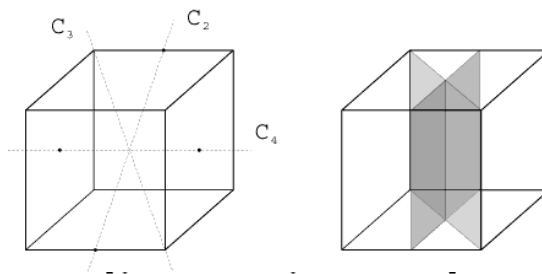
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Symmetry group example: O (cube)

- Inversion center I
 - Reflection planes
 - Rotation axes
- total: 24 elements (48 with i : O_h)



$3C_4, 3C_4^2, 3C_4^3, 4C_3, 4C_3^2, 6C_2$

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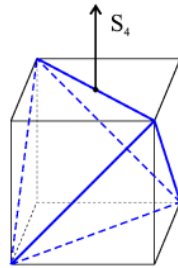
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Symmetry group example: O (cube)

- Inversion center /
- Reflection planes
- Rotation axes

total: 12 elements



T_d

$E, 3C_4^2, 4C_3, 4C_3^2, 3S_4, 3S_4^2, 6\sigma$

Notation for crystallographic directions and planes: Miller indices (see demonstration)

Crystal directions: $\vec{r}_n = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$ $[n_1 n_2 n_3]$

If there are several equivalent directions: $\langle n_1 n_2 n_3 \rangle$

Crystal planes:

If a plane intercepts the axes at x, y, z and basis vectors are a, b, c , then one can obtain three numbers

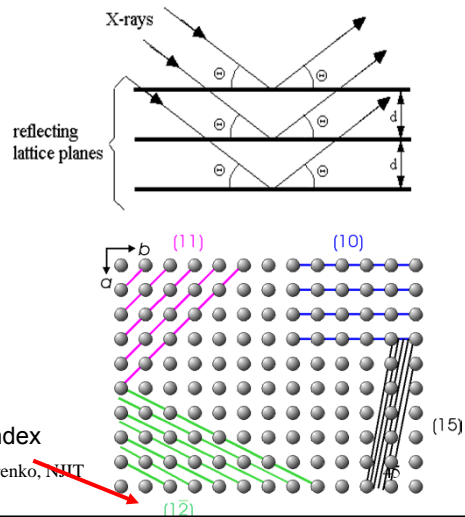
$$\left(\frac{a}{x}, \frac{b}{y}, \frac{c}{z} \right)$$

and reduce to the set of smallest integers (hkl) – *Miller indices* - represent a set of parallel planes

If there are several equivalent nonparallel sets of planes: $\{hkl\}$

Indexing system for crystal planes

- Since crystal structures are obtained from diffraction experiments (in which particles diffract from planes of atoms), it is useful to develop a system for indexing lattice planes.
- We can use the lattice constants a_1, a_2, a_3 , but it turns out to be more useful to use what are called Miller Indices.

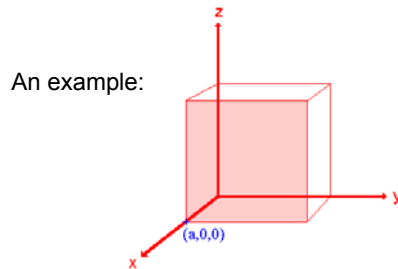


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Rules for determining Miller Indices

- (1) Find the intercepts on the axes in terms of the lattice constants a_1, a_2, a_3 .
- (2) Take the reciprocals of these numbers and then reduce to three integers having the same ratio, usually the smallest of the three integers. The result, listed as (hkl) , is called the index of the plane.



An example:

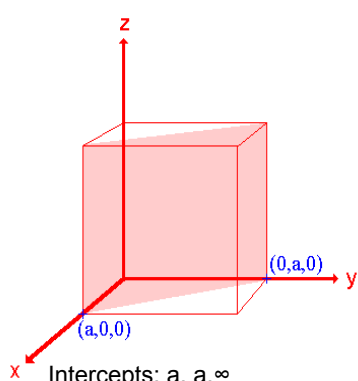
Intercepts: a, ∞, ∞
 Reciprocals: $a/a, a/\infty, a/\infty$
 $= 1, 0, 0$
 Miller index for this plane : $(1\ 0\ 0)$
 (note: this is the normal vector for this plane)

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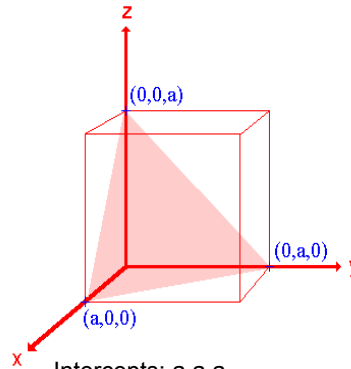
Examples of Miller Indices



Intercepts: a, a, ∞
 Reciprocals: $a/a, a/a, a/\infty$
 $= 1, 1, 0$
 Miller index for this plane : $(1\ 1\ 0)$

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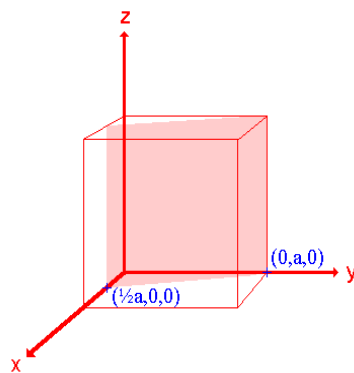
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Intercepts: a, a, a
 Reciprocals: $a/a, a/a, a/a$
 $= 1, 1, 1$
 Miller index for this plane : $(1\ 1\ 1)$

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Examples of Miller Indices



Intercepts: $1/2a, a, \infty$
 Reciprocals: $2a/a, a/a, a/\infty$
 $= 2, 1, 0$
 Miller index for this plane : $(2\ 1\ 0)$

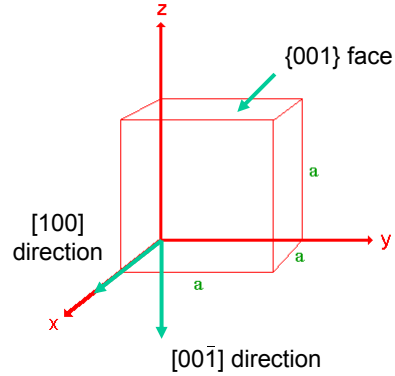
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Notes on notation

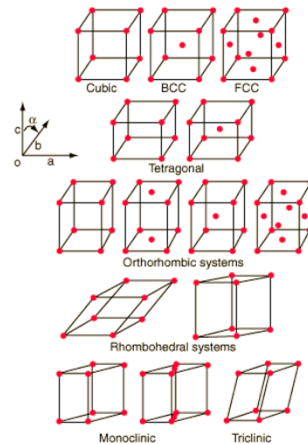
- (hkl) might mean a single plane, or a set of planes
- If a plane cuts a negative axis, we have minus signs in the (hkl) (ie. $(\bar{h}\bar{k}\bar{l})$)
- Planes are denoted with curly brackets $\{hkl\}$
- A set of faces are denoted $\{hkl\}$
- The direction of a crystal (for example, along x for a cubic crystal) is denoted with $[uvw]$ (ie. The $[100]$ direction)
- In cubic crystals, the direction $[hkl]$ is perpendicular to the plane (hkl) having the same indices, but this isn't necessarily true for other crystal systems



Summary

- A crystal lattice is a periodic array of the points related by translation operation: $\vec{r}_n = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$
- To form a crystal, we attach to every lattice point an identical group of atoms called basis
- 7 crystal systems and 14 Bravais lattices
- 32 crystal classes (point symmetry groups)
- Crystallographic directions and Miller indices; d_{hkl}

Continue with interatomic forces and types of bonds in solids



Reciprocal lattice

Constricting the reciprocal lattice from the direct lattice:

Let $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ - primitive vectors of the direct lattice; $\mathbf{T} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$

Then reciprocal lattice can be generated using the primitive vectors

$$\mathbf{b}_1 = \frac{2\pi}{V} \mathbf{a}_2 \times \mathbf{a}_3, \quad \mathbf{b}_2 = \frac{2\pi}{V} \mathbf{a}_3 \times \mathbf{a}_1, \quad \mathbf{b}_3 = \frac{2\pi}{V} \mathbf{a}_1 \times \mathbf{a}_2$$

where $V = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)$ is the volume of the unit cell

We have $\mathbf{b}_i \cdot \mathbf{a}_j = \delta_{ij}$

Some examples of reciprocal lattices

1. Reciprocal lattice to simple cubic lattice

$$\mathbf{a}_1 = a\mathbf{x}, \quad \mathbf{a}_2 = a\mathbf{y}, \quad \mathbf{a}_3 = a\mathbf{z} \quad V = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) = a^3 \Rightarrow$$

$$\mathbf{b}_1 = (2\pi/a)\mathbf{x}, \quad \mathbf{b}_2 = (2\pi/a)\mathbf{y}, \quad \mathbf{b}_3 = (2\pi/a)\mathbf{z} \quad \Rightarrow$$

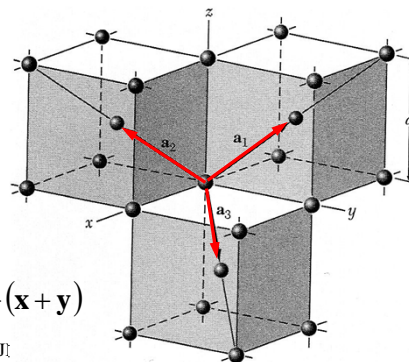
reciprocal lattice is also cubic with lattice constant $2\pi/a$

2. Reciprocal lattice to bcc lattice

$$\mathbf{a}_1 = \frac{1}{2}a(-\mathbf{x} + \mathbf{y} + \mathbf{z}) \quad \mathbf{a}_2 = \frac{1}{2}a(\mathbf{x} - \mathbf{y} + \mathbf{z})$$

$$\mathbf{a}_3 = \frac{1}{2}a(\mathbf{x} + \mathbf{y} - \mathbf{z}) \quad V = |\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3| = \frac{1}{2}a^3$$

$$\Rightarrow \mathbf{b}_1 = \frac{2\pi}{a}(\mathbf{y} + \mathbf{z}) \quad \mathbf{b}_2 = \frac{2\pi}{a}(\mathbf{x} + \mathbf{z}) \quad \mathbf{b}_3 = \frac{2\pi}{a}(\mathbf{x} + \mathbf{y})$$

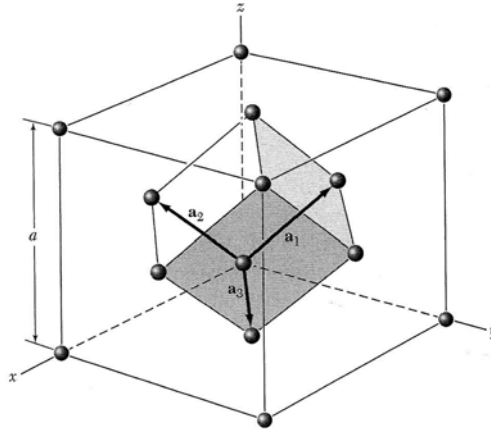


got $\mathbf{b}_1 = \frac{2\pi}{a}(\mathbf{y} + \mathbf{z})$

$\mathbf{b}_2 = \frac{2\pi}{a}(\mathbf{x} + \mathbf{z})$

$\mathbf{b}_3 = \frac{2\pi}{a}(\mathbf{x} + \mathbf{y})$

but these are primitive vectors of fcc lattice



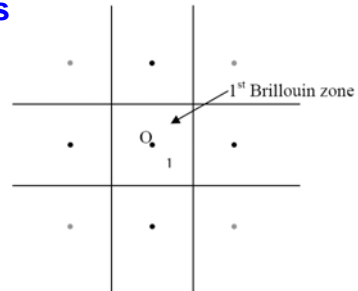
So, the reciprocal lattice to bcc is fcc.

Analogously, show that the reciprocal lattice to fcc is bcc

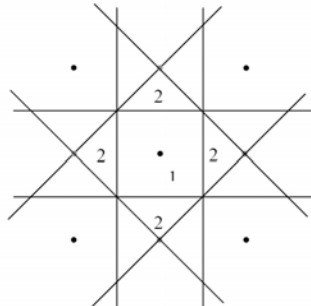
Brillouin zones

Determine all the perpendicular bisecting planes in the reciprocal lattice

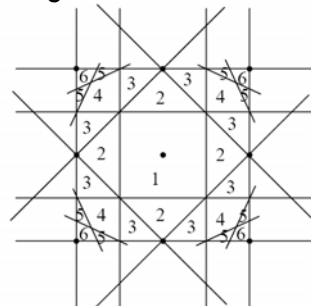
First Brillouin zone - the Wigner-Seitz cell of the reciprocal lattice



Second Brillouin zone:

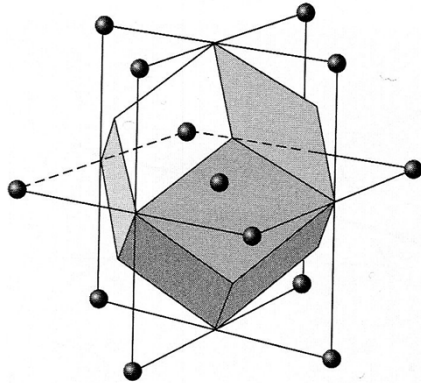


Higher Brillouin zones:

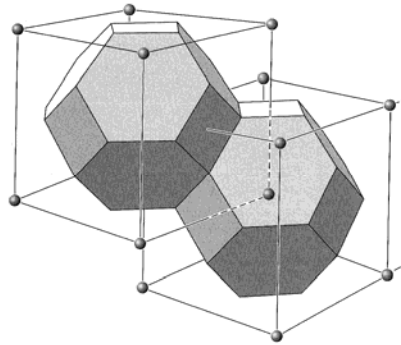


Brillouin zones of cubic lattices

First BZ of a BCC lattice



First BZ of an FCC lattice



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Summary

- ❖ Reciprocal lattice is defined by primitive vectors:

$$\mathbf{b}_1 = \frac{2\pi}{V} \mathbf{a}_2 \times \mathbf{a}_3, \quad \mathbf{b}_2 = \frac{2\pi}{V} \mathbf{a}_3 \times \mathbf{a}_1, \quad \mathbf{b}_3 = \frac{2\pi}{V} \mathbf{a}_1 \times \mathbf{a}_2$$

- ❖ A reciprocal lattice vector has the form $\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$
It is normal to (hkl) planes of direct lattice
- ❖ First Brillouin zone is the Wigner-Seitz primitive cell of the reciprocal lattice
- ❖ Simple cubic \rightarrow cube; bcc \rightarrow Rhombic dodecahedron;
fcc \rightarrow truncated octahedron (figures on the previous slide)

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We already know:

- crystal lattice; 7 crystal systems; 14 Bravais lattices
- 32 point symmetry groups (crystal classes)
- Crystallographic directions and Miller indices; d_{hkl}

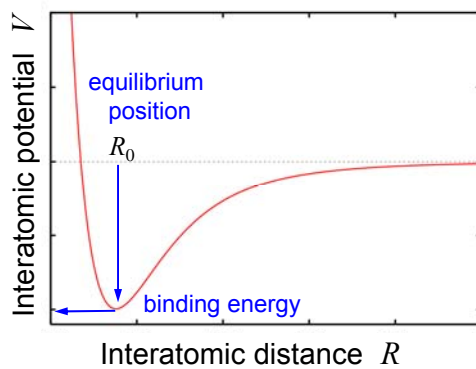
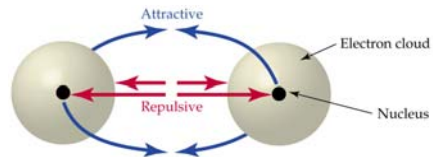
CONTINUE with:

Inter-atomic forces and types of bonds in solids.

Interatomic forces

What holds a crystal together?

Attractive electrostatic interaction between electrons and nuclei – the force responsible for cohesion of solids



Force:

$$F(R) = -\frac{\partial V(R)}{\partial R}$$

$F(R) < 0$ for $R > R_0$:
attraction

$F(R) > 0$ for $R < R_0$:
repulsion

Types of bonding

I. Ionic crystals

Usually involve atoms of strongly different electro-negativities
(Example: alkali halides).

$$U(R) = -N \frac{\alpha e^2}{4\pi\epsilon_0 R} + N \frac{A}{R^n}$$

attractive
(Coulomb)

repulsive

Ionic bond is strong
(binding energy - few eV/pair)

⇒ hardness, high melting T

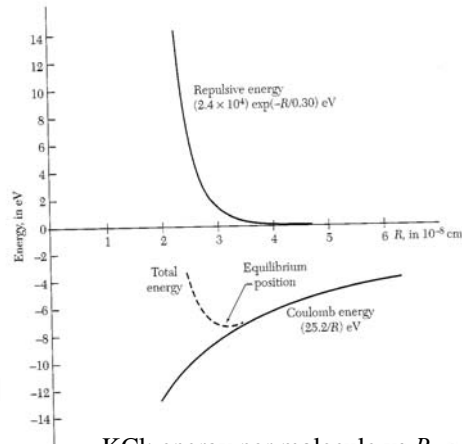
electrons are strongly localized

⇒ insulators in solid form

Typical crystal structures: NaCl, CsCl

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KCl: energy per molecule vs R
(from Kittel)

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II. Covalent crystals

- Electron pair bond: usually one electron from each atom
- Electrons tend to be localized in part between the two atoms
- The spins of electrons in the bond are anti-parallel
- Gap between fully occupied and unoccupied states → dielectrics or semiconductors

Directionality of covalent bonds. Example: carbon

Hybridization. $2s^2 2p^2 \rightarrow 2s 2p_x 2p_y 2p_z$: sp^3 tetrahedral configuration

Also possible sp^2 : $2s 2p_x 2p_y$ – planar (graphite, fullerenes)
remaining p_z : interlayer π -bonding

Covalent polar bond (many compound semiconductors) –
intermediate case between non-polar and ionic bond. Described by
effective ionic charge or fractional ionic character (between 0 and 1:
0 for Si or diamond, 0.94 for NaCl). Covalent bond is also strong,
binding energies of several eV per atom

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III. Metals

- Most elements in periodic table
- High electrical and thermal conductivity
- High density
- Considerable mechanical strength, but plasticity

These properties can be explained considering the metallic type of bond

Example: alkali metals – single electron weakly bound to atom – easily delocalized.

In contrast to covalent bonding, electronic wave functions are very extended compared to interatomic distances. Why total energy is reduced ?

Partially occupied electronic bands – electrons can move freely

Group II metals – two *s* electrons – should be fully occupied...
but overlapped with empty *p*-states

Transition metals: *d*-electrons are more localized – form covalent-like bonds; *s* and *p*-electrons again form a common band

Metals crystallize in closely packed structures (hcp, fcc, bcc)

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IV. Van der Waals bonds

Inert gases: outer electronic shells are full – no ionic or covalent forces

Weak interatomic forces due to quantum fluctuations of charge → arising dipole moments cause a weak attractive force

Can be described in the quantum-mechanical model of two linear oscillators (given in Kittel) → results in R^{-6} dependence of potential

Binding energy in order of 0.1 eV

Crystal structures are fcc (electronic distribution is spherical, atoms pack as closely as possible)

Van der Waals forces are also responsible for bonding in organic molecular crystals. Molecules are weakly bound; often form low-symmetry crystals

They also exist in covalent or ionic crystals, but negligible

V. Hydrogen bonds

Formed between two strongly electronegative atoms (F, O, N) via H

Example: ice

Binding energy is also ~0.1 eV

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Summary

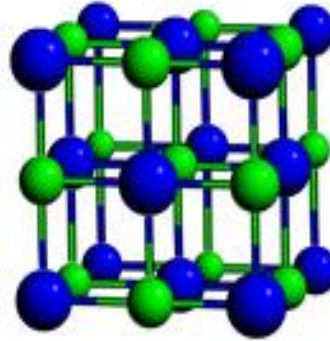
- ❖ Repulsive interaction between atoms is primarily due to electrostatic repulsion of overlapping charge distributions and Pauli principle
- ❖ Several types of attractive forces:
 - Ionic crystals – electrostatic forces between "+" and "-" ions
 - Covalent bond: overlap of charge distributions with antiparallel spin
 - Metals: reduction of kinetic energy of electrons in free state compared to the localized state of a single atom
 - Secondary forces (Van der Waals, hydrogen) become significant when the other bonds are impossible, e.g. in inert gases
- ❖ Physical properties are closely related to the type of bonding

Condensed Matter Physics Crystals (continued)

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Examples of common structures:
 (1) The Sodium Chloride (NaCl) Structure (LiH, MgO, MnO, AgBr, PbS, KCl, KBr)

- The NaCl structure is FCC
- The basis consists of one Na atom and one Cl atom, separated by one-half of the body diagonal of a unit cube
- There are four units of NaCl in each unit cube
- Atom positions:
- Cl : 000 ; $\frac{1}{2}\frac{1}{2}0$; $\frac{1}{2}0\frac{1}{2}$; $0\frac{1}{2}\frac{1}{2}$
- Na: $\frac{1}{2}\frac{1}{2}\frac{1}{2}$; $00\frac{1}{2}$; $0\frac{1}{2}0$; $\frac{1}{2}00$
- Each atom has 6 nearest neighbours of the opposite kind



Often described as 2 interpenetrating FCC lattices

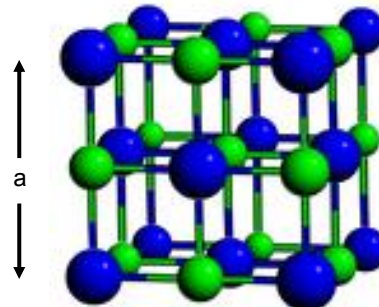
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NaCl structure

Crystal	a
LiH	4.08 Å
MgO	4.20
MnO	4.43
NaCl	5.63
AgBr	5.77
PbS	5.92
KCl	6.29
KBr	6.59



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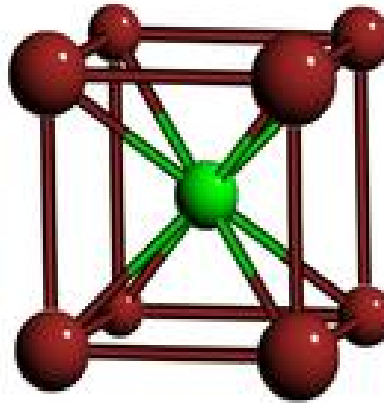
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(2) The Cesium Chloride (CsCl)

structure

(CsBr, CsI, RbCl, AlCo, AgZn, BeCu, MgCe, RuAl, SrTi)

- The CsCl structure is BCC
- The basis consists of one Cs atom and one Cl atom, with each atom at the center of a cube of atoms of the opposite kind
- There is one unit of CsCl in each unit cube
- Atom positions:
- Cs : 000
- Cl : $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ (or vice-versa)
- Each atom has 8 nearest neighbors of the opposite kind



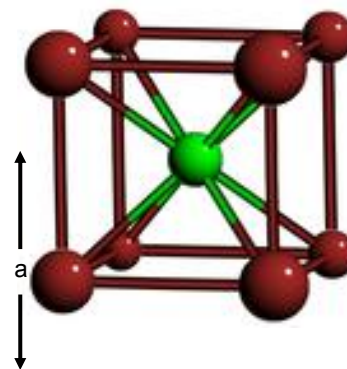
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CsCl structure

Crystal	a
BeCu	2.70 Å
AlNi	2.88
CuZn	2.94
CuPd	2.99
AgMg	3.28
LiHg	3.29
NH ₄ Cl	3.87
TlBr	3.97
CsCl	4.11
TlI	4.20



Why are the a values smaller for the CsCl structures than for the NaCl (in general)?

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