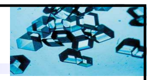
Lecture 1



1.1 Crystal Lattices
1.2 The Reciprocal Lattice
1.3 Experimental Determination of Crystal Structure

Crystal:
a solid composed of atoms, ions, or molecules arranged in a pattern that is repeated in three dimensions
A material in which atoms are situated in a repeating or periodic array over large atomic distances

References:
1. Marder, Chapters 1-3
2. Kittel, Chapter 1 and 2
3. Ashcroft and Mermin, Chapter 4-6
4. Burns, Chapters 1-2
5. Ziman, Chapter 1

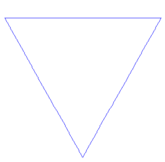
- **Crystalline materials**
 - atoms (ions or molecules) in repeating 3D pattern (a lattice)
 - long-range order; ex.: NaCl,

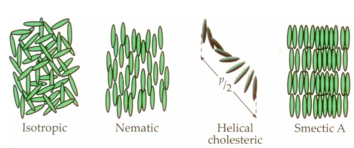
- **Amorphous (noncrystalline) materials**
- **Short range order, not periodic; ex.: liquid water, glass**

- **Fractals**
- long-range order, symmetry, but not repeating

- **Liquid crystals**
- **long range order of one type; disorder of another**
- **nematic and smectic**

Fractals **Liquid crystals**

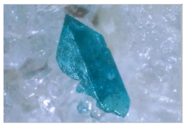
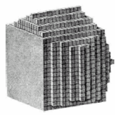
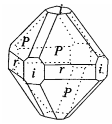




1.1 Crystal Lattices

Atomic Structure Questions:
- What is the basic structure of matter?
- How do atoms spontaneously organize?

Basic Answers:
- Scaling theory relates atom-scale units to macroscopic solids
- Atoms form crystalline arrays
- Idea comes from special class of solids: minerals

See vast numbers of minerals at http://webmineral.com/

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1.1.1 Two-Dimensional Lattices

Definitions:
- Bravais lattice
- Primitive vector
- Basis vector
- Unit cell (primitive or not)
- Wigner-Seitz cell (Voronoi polyhedron)
- Translation, space and point groups

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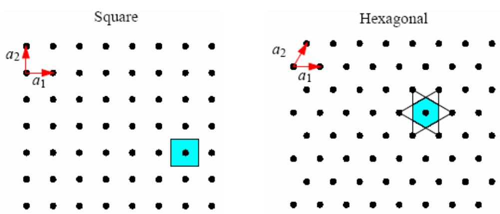
Bravais Lattices



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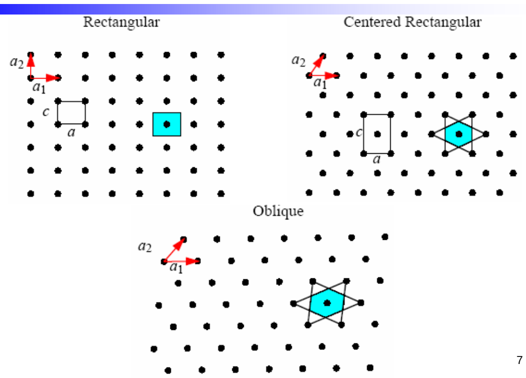
Bravais Lattices



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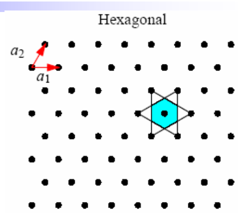
Questions

Are primitive vectors unique?

No

For hexagonal lattice $\vec{a}_1 = a(1\ \ 0)$

$$\vec{a}_2 = a(\frac{1}{2}\ \ \frac{\sqrt{3}}{2})$$



We can also choose $\vec{a}_{1,alt} = a(-\frac{1}{2}\ \ \frac{\sqrt{3}}{2})$

$$\vec{a}_{2,alt} = a(\frac{1}{2}\ \ \frac{\sqrt{3}}{2})$$

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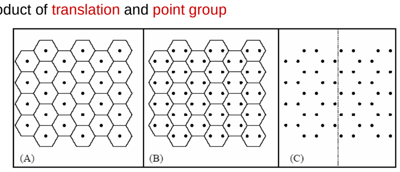
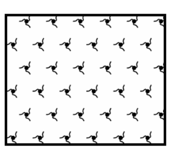
Lattice with Basis

Note presence of glide plane, showing that space group is not the same as the product of translation and point group



Some, but not all symmetries of triangular lattice destroyed



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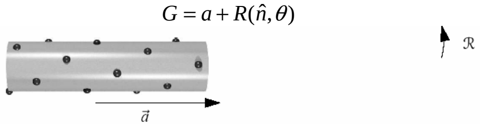
Symmetries and The Space Group

The complete set of rigid body motions that takes a crystal into itself is called **space group**

$$G = a + R(\hat{n}, \theta)$$



Two subgroups: translation and point groups

Translation: translation through all lattice vectors defined by $n_1\vec{a}_1 + n_2\vec{a}_2 + \ldots$

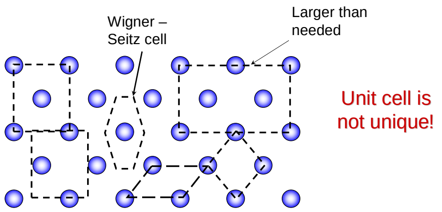
and it leaves the crystal unchanged (invariant)

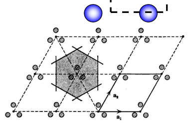
Point group consists of rotations that leave the crystal invariant

… plus crew axis and glide planes

Summary: Classification of 2D periodic Structures

Unit cell: a convenient repeating unit of a crystal lattice; the axial lengths and axial angles are the lattice constants of the unit cell





Wigner – Seitz Cell : place the symmetry centre in the centre of the cell; draw the perpendicular bisector planes of the translation vectors from the chosen centre to the nearest equivalent lattice site

Questions

How many distinct Bravais lattices are there?

Five

How many distinct two-dimensional lattices are there?

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http://www2.spsu.edu/math/tile/symm/ident17.htm

1.1.2 Three–Dimensional Crystals

- Distribution of structures among elements
- A small number of popular crystal structures
- Crystal symmetries:
  - 7 **crystal systems**
  - 14 **Bravais lattices**
  - 32 **point groups**
  - 230 **space groups**

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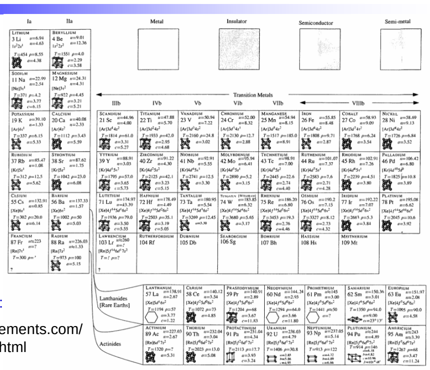
Crystallization of Pure Elements

From Marder:



Web of Elements:

http://www.webelements.com/crystal_structure.html

Allotropy

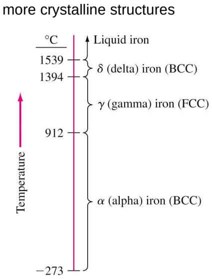
Allotropy – the ability of element to exist in two or more crystalline structures

Fe: bcc ⇒ fcc ⇒ bcc

In case of compound it is called **polymorphism**

Carbon allotropic forms: ?

- diamond
- graphite
- fullerene or buckyballs
- nanotubes or buckysheets



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Allotropy

Many elements adopt multiple crystal structures between 0 K and their melting temperatures

Plutonium has a rich phase diagram

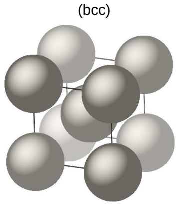
Transformation Temp, C	Phase	Structure (atoms per unit cell)	Density (g/cc)
112	α	monoclinic (16)	19.8
185	β	fc monoclinic (34)	17.8
310	γ	fc orthorhombic (8)	17.1
450	δ	fcc (4)	15.9
475	δ'	fc tetragonal (2)	16.0
640	ϵ	bcc (2)	16.5

Table 1: Source, Atomic Weapons Establishment, Discovery Article

Popular Lattices

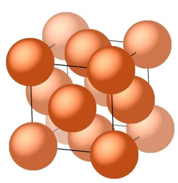
>90% of elemental metals crystallize upon solidification into **3** densely packed crystal structures:

Body-centered cubic (bcc)



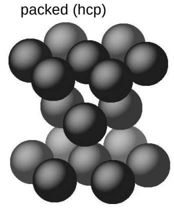
ex.: Fe, W, Cr

Face-centered cubic (fcc)



ex.: Cu, Ag, Au

Hexagonal close-packed (hcp)



ex.: Zr, Ti, Zn

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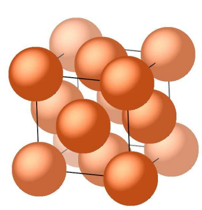
Important to know:

- **Distance between atoms (d)**
  - in terms of *a*
- **Number of atoms in the unit cell**
  - each corner atoms shared by 8 cells: 1/8
  - each face atom shared by 2 cells: ½
  - each edge atom shared by 4 cells: ¼



- **Coordination number**
  - Number of nearest neighbours (n.n.); for metals all equivalent
- **Atomic Packing Factor (APF)**

APF = Volume of atoms in unit cell / Volume of unit cell (a^3)

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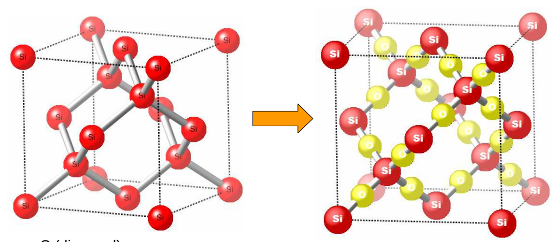
Diamond and Silicon dioxide



C (diamond)
Si, Ge

Cristobalite (SiO_2)
Si C.N. = 4 SiO_4^{4-}
O C.N. = 2

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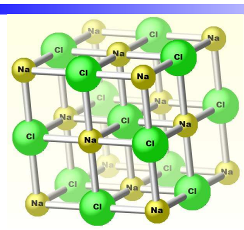
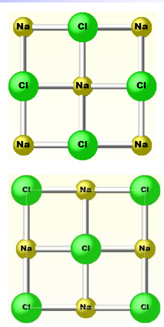
Sodium Chloride – NaCl (Rocksalt)





Layer 1

Layer 2

Layer 3 = Layer 1

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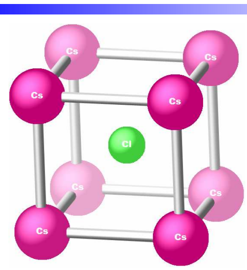
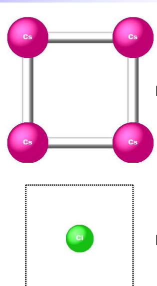
Cesium Chloride - CsCl



Cs (0, 0, 0)
Cl (1/2, 1/2, 1/2)



Layer 1

Layer 2

Layer 3 = Layer 1

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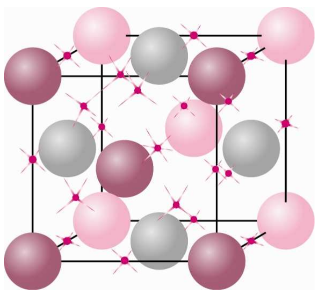
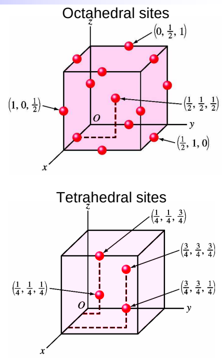
Interstitial Sites in *fcc* Crystal Lattice





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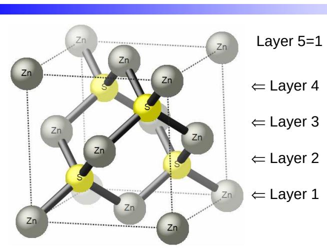
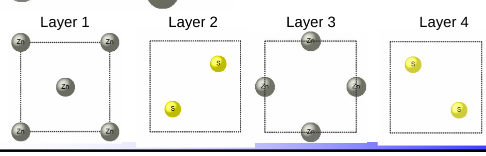
Zinc Blend (ZnS) crystal structure



Zn (0, 0, 0)

S (x+0.25, y+0.25, z+0.25)



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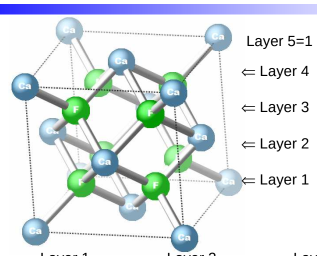
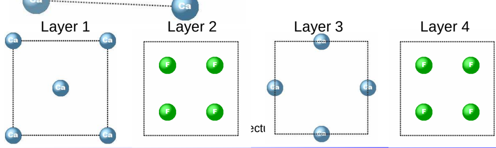
Calcium Fluoride – CaF_2



Ca (0, 0, 0)

F (+0.25, +0.25, +0.25)

(-0.25, -0.25, -0.25)



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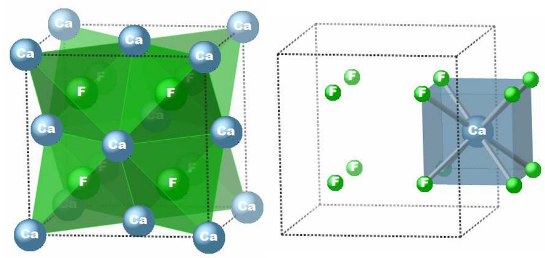
CaF_2 - coordination



CO_2, CdF_2, CeO_2, $CoSi_2$, ZrO_2

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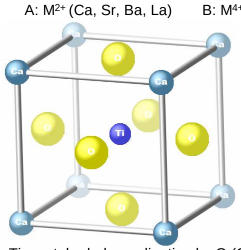
Perovskite – $CaTiO_3$

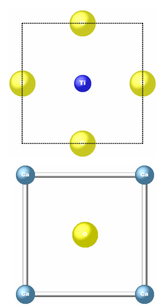
ABO_3

A: M^{2+} (Ca, Sr, Ba, La) B: M^{4+} (Ti, Zr, Mn)



Layer 2: TiO_2

Layer 1: CaO



Ti – octahedral coordination by O (CN=6)
d(Ti-O)= *a* / 2
Ca – cuboid coordination by O (CN = 12)
O – octahedral by Ti and Ca

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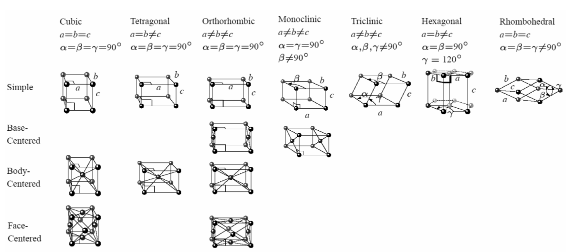
14 Bravais Lattices and 7 Crystal Systems



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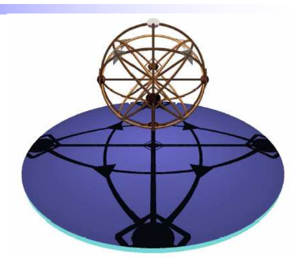
Symmetry Elements

Symmetry of Lattices

Axis type	Schönflies Notation	International Notation	Symbol	Operation
Inversion	$i = S_2$	$\bar{1}$		$\vec{r} \rightarrow -\vec{r}$
Twofold	C_2	2	or	
Threefold	C_3	3	or	
Fourfold	C_4	4		
Sixfold	C_6	6		
Twofold Rotoinversion or Mirror	σ_h, $\perp$ to axis σ_v, plane contains axis $\bar{2} \equiv m$ σ_d, bisects twofold axes		or	
Threefold Rotoinversion	S_6^{-1}	$\bar{3}$		
Fourfold Rotoinversion	S_4^{-1}	$\bar{4}$		
Sixfold Rotoinversion	S_3^{-1}	$\bar{6}$		



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Schönflies and International Notations

Schönflies

C = Cyclic; allows successive rotation about main axis.

D = Dihedral; contains two-fold axes perpendicular to main axis.

S = Spiegel; unchanged after combination of reflection and rotation.

T = Tetragonal.

O = Octahedral.

A subscript *n=1 …6* denotes the order of a rotational axis, and subscripts denote the three types of mirror plane on previous slide

International

Associates each group with a list of its symmetry axes.

Notation such as *6m* refers to a mirror plane containing a six-fold axis, while *6/m* refers to a mirror plane perpendicular to the six-fold axis

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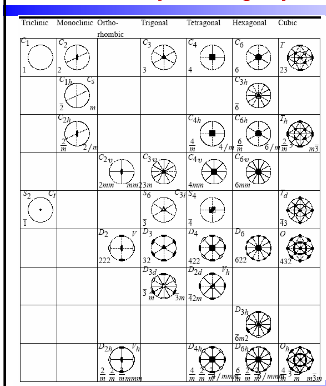
32 Crystallographic Point Groups



Learn more here:

http://www.uwgb.edu/dutchs/SYMMETRY/3dSpaceGrps/3DSPGRP.HTM

http://www.ccas.ru/galiulin/feddos1.html

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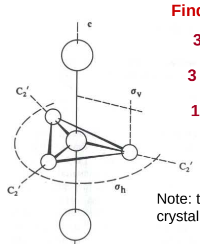
Symmetry Operations

- **Symmetry operation** for a molecule or crystal is an operation that interchanges the positions of the various atoms in such a way that the molecule or crystal appear exactly as before the operation



Find of the symmetry operations:

3 rotations around P-F axis

3 mirror planes Cl, P and different F atoms

1 mirror plane with P and F atoms

rotation by 120º and 240º around *c*-axis

identity operation

Note: the axis of highest symmetry of a molecule or crystal is called the **principle axis** or **c-axis** or **z-axis**

HW task #1: draw a stereogram for PF_3Cl_2

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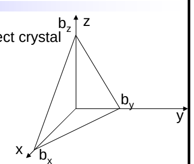
Bulk Truncation Structure

Ideal flat surface: truncating the bulk structure of a perfect crystal



Miller Indices, revisited

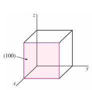
- For plane with intersections at b_x, b_y b_z

write reciprocals: $\left(\frac{1}{b_x}\frac{1}{b_y}\frac{1}{b_z}\right)$

- If all quotients are rational integers or 0, this is Miller index

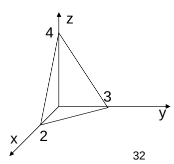
e.g., b_x, b_y, b_z = 1, 1, 0.5 $\Rightarrow$ (112)

b_x, b_y, b_z = 1, ∞, ∞ $\Rightarrow$ (100)



- In general

Miller index $(i,j,k)=\left(\frac{cd}{b_x}\frac{cd}{b_y}\frac{cd}{b_z}\right)$, where cd - common denom. of b_x, b_y, b_z



e.g., $cd=12;\ (i,j,k)=\left(\frac{12}{2}\frac{12}{3}\frac{12}{4}\right)=(643)$:ture 1

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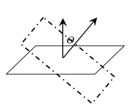
Angles between the planes

$$[ijk]=[lmn]\times[opq]$$



Cross products of two vectors in a plane defines direction perpendicular to plane

[*lmn*] and [*opq*] are both vectors in plane (*ijk*)

Angle between two planes (directions) $\cos\Theta=\frac{[ijk]\bullet[lmn]}{\sqrt{i^2+j^2+k^2}\sqrt{l^2+m^2+n^2}}$

e.g., for [111], [211] : $\cos\Theta=\frac{2+1+1}{\sqrt{3}\sqrt{6}}\Rightarrow\Theta=19.47^o$

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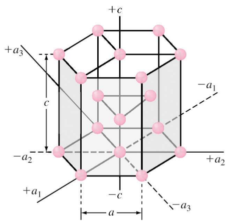
Planes in hexagonal crystals

4 coordinate axes (a_1, a_2, a_3, and c) of the HCP structure (instead of 3)

Miller-Bravais indices - (h k i l) – based on 4 axes coordinate system



a_1, a_2, and a_3 are 120º apart: h k i

c axis is 90º: l

3 indices (rarely used):

$h + k = - l$

$(h\ k\ i\ l) \Rightarrow (h\ k\ l)$

Note: in hcp, (001) ≠(100)

Basal and Prizm Planes

Basal planes;

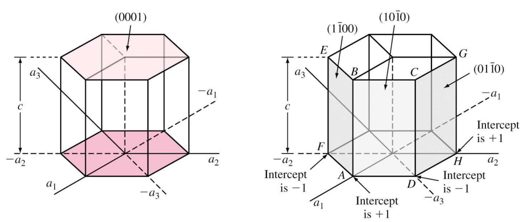
$a_1 = \infty$; $a_2 = \infty$; $a_3 = \infty$; $c = 1$

⇒ (0 0 0 1)

Prizm planes: ABCD

$a_1 = +1$; $a_2 = \infty$; $a_3 = -1$; $c = \infty$

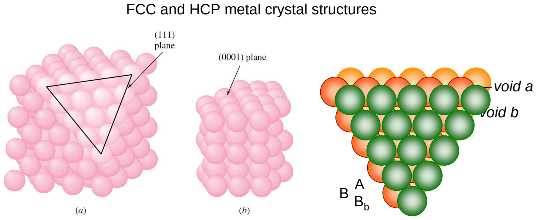
⇒ (1 0 -1 0)



(a) (b)

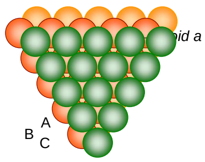
Comparison of crystal structures

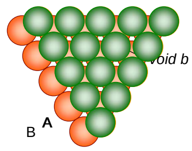
FCC and HCP metal crystal structures



- (111) planes of fcc have the same arrangement as (0001) plane of hcp crystal
- 3D structures are not identical: stacking has to be considered

FCC and HCP crystal structures





fcc

B plane placed in *a* voids of plane A

Next plane placed in *a* voids of plane B, making a new C plane

Stacking: ABCABC…

hcp

B plane placed in *a* voids of plane A

Next plane placed in *a* voids of plane B, making a new A plane

Stacking: ABAB…

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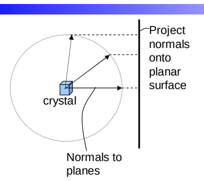
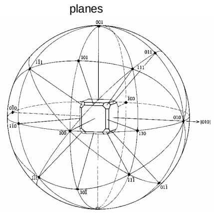
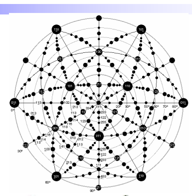
Stereographic Projections







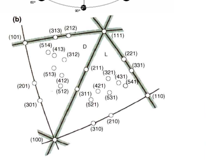


Figure 1.12 Stereogram projected on (001) showing the mirror zones relevant to primitive fcc, bcc and simple cubic crystal surfaces. Note that right-handed axes are used. The chiralities of two triangles are labelled D and L according to the symmetry-based convention of Pratt et al.[51] Reproduced from S.J. Pratt et al., *Surf. Sci.*, **585**, L159. Copyright (2005), with permission from Elsevier.

from K.Kolasinski

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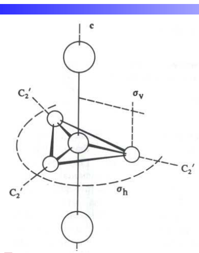
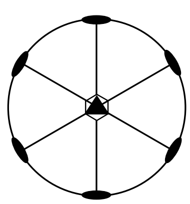
Stereogram for PF_3Cl_2





E
C_3, C_3^2
3 C_2'
σ_h
3 σ_v
S_3, S_3^5

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1.2 Reciprocal Space

Reciprocal space is also called **Fourier** space, ***k***- space, or **momentum** space in contrast to real space or direct space

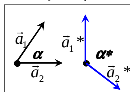
The **reciprocal space** lattice is a set of imaginary points constructed in such a way that the direction of a vector from one point to another coincides with the direction of a normal to the real space planes and the separation of those points (absolute value of the vector) is equal to the reciprocal of the real interplanar distance

⇒ The things which are larger in real space are smaller in *reciprocal space* by definition

1.2 Reciprocal Space Lattices

- Given a unit cell with basis vectors $(\vec{a}_1, \vec{a}_2)$
- There is a complementary reciprocal lattice $(\vec{a}_1^*, \vec{a}_2^*)$

$\vec{a}_i \cdot \vec{a}_j^* = \delta_{ij} \quad (i, j = 1, 2) \Rightarrow \vec{a}_1^* \perp \vec{a}_2$ and $\vec{a}_2^* \perp \vec{a}_1$

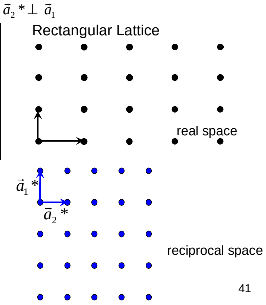


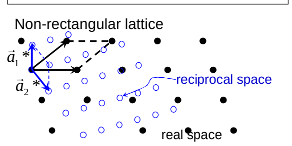
Area of unit cell A

$A = |\vec{a}_1||\vec{a}_2|\sin\alpha$

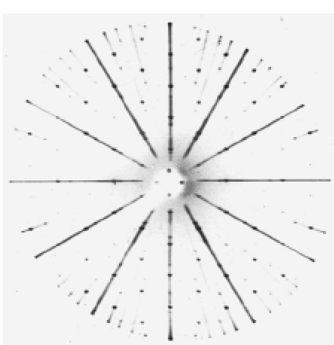
$A^* = |\vec{a}_1^*||\vec{a}_2^*|\sin\alpha^*$

$A^* = \frac{1}{A}$





1.3 Experimental Determination of Crystal Structures



History

Experiments and theory in 1912 finally revealed locations of atoms in crystalline solids

Essential ingredients:

- Theory of diffraction grating
- Skiing, and physics table at Café Lutz
- X-ray tubes, photographic plates, and first experiments with their use
- Persistence
- Coherent experiments with incoherent theory along behind

Incident particles to consider:

X-rays
Neutrons
Electrons ?
Atoms ?

	X-rays	Neutrons	Electrons
Charge	0	0	$-e$
Mass	0	$1.67 \cdot 10^{-27}$ kg	$9.11 \cdot 10^{-31}$ kg
Typical energy	10 keV	0.03 eV	100 keV
Typical wavelength	1Å	1 Å	0.05Å
Typical attenuation length	100 μm	5 cm	1 μm
Typical atomic form factor, f	10^{-3} Å	10^{-4} Å	10 Å

Term

- Miller indices
- Reciprocal lattice

Structure Determination

- Bragg scattering, elastic and inelastic
- Bragg angle, Bragg peak and crystal planes

- Atomic form factor
- Structure factor
- Extinctions

Experimental Methods:

- Ewald construction
- Laue method
- Debye-Scherrer method, powder diffraction

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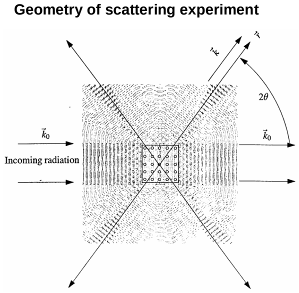
Theory of Scattering from Crystals

Geometry of scattering experiment



Elastic scattering: frequency of outgoing radiation is the same as that of incoming

Radiation of wave vector $\vec{k}_o$ arrives at a sample, introducing a circular ring of radiation from each atom

If k_o is chosen just right, the scattering radiation from the atoms adds constructively in certain directions

X-ray – EM

n, e - QM

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Scattering from a particle

At the origin

Schiff, page 115 or Jackson Eq. 9.8

$$\psi \approx Ae^{-i\omega t}[e^{i\vec{k}_o\vec{r}} + f(r)\frac{e^{ik_o r}}{r}]$$

$$I_{atom} = \frac{d\sigma}{d\Omega_{atom}} = |f(r)|^2$$

f is atomic **form factor**

Contains details of interactions between the scattering potential and the scattered wave

Let's assume we know $f(r)$

At $\vec{R}$

$$\psi \sim Ae^{-i\omega t}e^{i\vec{k}_o\vec{R}}[e^{i\vec{k}_o(\vec{r}-\vec{R})} + f(r)\frac{e^{i\vec{k}_o(\vec{r}-\vec{R})}}{|\vec{r}-\vec{R}|}]$$

For sufficiently large r,

$$\vec{k}_o(\vec{r}-\vec{R}) \sim k_o r - k_o\frac{\vec{r}}{r}\vec{R}$$

Using Eq. above and defining $\vec{k} = k_o\frac{\vec{r}}{r}$ and $\vec{q} = \vec{k}_o - \vec{k}$

$$\psi \sim Ae^{-i\omega t}[e^{i\vec{k}_o\vec{r}} + f(r)\frac{e^{ik_o r + i\vec{q}\vec{R}}}{r}]$$

$q = 2\,k_0 \sin\theta$

$\hbar\vec{q}$ - *momentum transfer between incoming and outgoing waves*

θ - Bragg angle

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Scattering Theory

Coherent scattering pattern reveals crystalline pattern

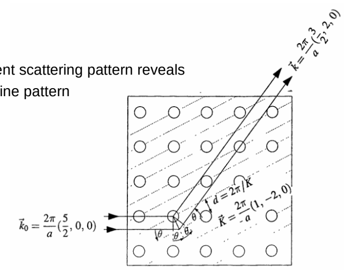

Illustration of Bragg scattering at angle θ = 26.56° from the (21) planes of a square lattice. The magnitudes of $\mathbf{k}_o$, **k**, and **K** are determined using Eqs. (3.38) and (3.39), Marder.

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Many scattering particles

Assuming multiple scattering and inelastic scattering can be ignored

$$\psi \sim Ae^{-i\omega t}[e^{i\vec{k}_o\vec{r}} + \sum_l f_l(r)\frac{e^{i\vec{k}_o\vec{r} + i\vec{q}\vec{R}_l}}{r}]$$

In direction away from incident beam

$$\psi \sim Ae^{-i\omega t}[\sum_l f_l(r)\frac{e^{i\vec{k}_o\vec{r} + i\vec{q}\vec{R}_l}}{r}]$$

Intensity per unit solid angle

$$I = \sum_{l,l'} f_l f_{l'}^* e^{i\vec{q}(\vec{R}_l - \vec{R}_{l'})}$$

Equation above is true no matter how atoms are arranged!

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Scattering from crystal

If all of the scatters are identical and arranged in a Bravais lattice:

$$I = I_{atom}\left|\sum_{l} e^{i\vec{q}\vec{R}_l}\right|^2$$

Laue condition : find $\vec{q}$ so that for all atom locations $\vec{R}_l$

$$e^{i\vec{q}\vec{R}_l} = 1$$

One-Dimensional Sum: lattice points must be of the form *la*

$$\sum_q = \sum_{l=0}^{N-1} e^{ilaq}$$

(follow Marder, p. 48)

$$\sum_q = \frac{e^{iNaq}-1}{e^{iaq}-1}; \quad \left|\sum_q\right|^2 = \frac{\sin^2 \frac{Naq}{2}}{\sin^2 \frac{aq}{2}}$$

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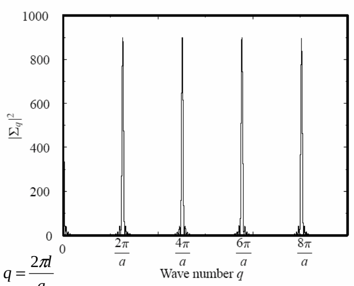
Scattering for one-dimension



Peak when

$$\frac{aq}{2} = l\pi \Rightarrow q = \frac{2\pi l}{a}$$

Assuming delta functions:

$$\sum_{l=0}^{N-1} e^{ilaq} = \sum_{l'=-\infty}^{N-1} N\frac{2\pi}{L}\delta(q - \frac{2\pi l'}{a})$$

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Scattering in three dimensions

Main result : when $\vec{q} = \vec{k}_o - \vec{k} = \vec{K}$ satisfies

$e^{i\vec{K}\vec{R}} = 1$ or $\vec{K}\cdot\vec{R} = 2\pi l$

there is a strong peak

The scatering sum can be rewritten

$$\sum_{\vec{R}} e^{i\vec{R}\vec{q}} = \sum_{\vec{K}} N\frac{(2\pi)^3}{V}\delta(\vec{q} - \vec{K})$$

When the vectors **R** lie in a Bravais lattice, then vectors **K** satisfying equation above also lie in a lattice – the reciprocal lattice

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Lattice with a Basis

$$\vec{R} = \vec{u}_l + \vec{v}_{l'}$$

Regrouping of basic sum first carried out by Laue

$$\begin{aligned}\sum_{\vec{R}} e^{i\vec{q}\cdot\vec{R}} &= \sum_{ll'} e^{i\vec{q}\cdot(\vec{u}_l+\vec{v}_{l'})} \\ &= \left(\sum_l e^{i\vec{q}\cdot\vec{u}_l}\right)\left(\sum_{l'} e^{i\vec{q}\cdot\vec{v}_{l'}}\right) \\ \Rightarrow I &\propto \left(\sum_{jj'} e^{-i\vec{q}\cdot(\vec{u}_j-\vec{u}_{j'})}\right)\left(\sum_{ll'} e^{i\vec{q}\cdot(\vec{v}_l-\vec{v}_{l'})}\right).\end{aligned}$$

Structure factor for the unit cell is

$$F_{\vec{q}} \equiv |\sum_l e^{i\vec{q}\cdot\vec{v}_l}|^2.$$

When $F_{\vec{q}}$ vanishes, have an extinction: Laue overlooked this possibility, leading to years of confusion interpreting patterns.

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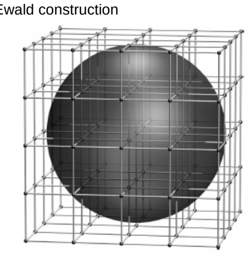
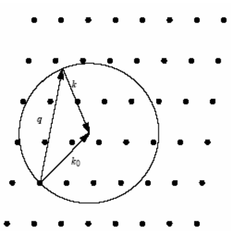
Experimental Methods

Ewald construction





Shining generic monochromatic X-ray upon crystal gives no scattering peaks!!!

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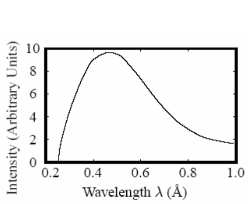
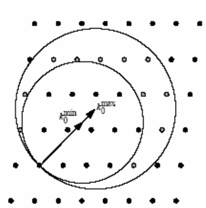
Laue Method





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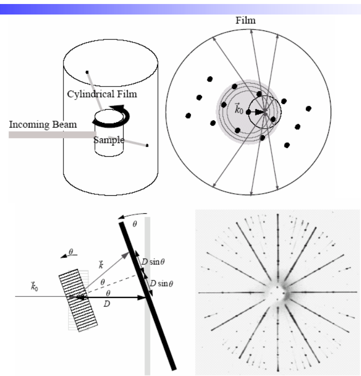
Rotating Crystal Method



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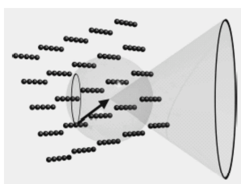
Powder Diffraction



$$\theta = \sin^{-1}\left(\frac{K}{2k_o}\right)$$

And the radius r on film of the scattering ring due to the reciprocal lattice vector **K** is

$$r = D\tan(2\theta)$$

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Powder diffraction

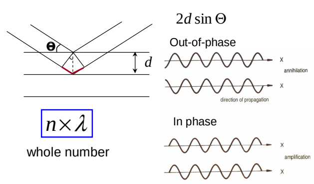
<u>Main method for determining crystal structure</u>

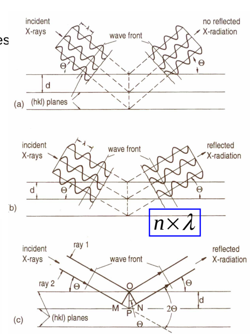
Consider an X-ray of wavelength λ hits a set of planes separated by d under an angle Θ

- some of the X-rays go straight through

- some are reflected (scattered), but only if specific conditions met

Consider a material to be a stack of planes at a constant separation - d





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Bragg's law

The diffraction (the coherent elastic scattering of waves by the crystal lattice) condition

$$n \times \lambda = 2d \sin\Theta$$

Bragg's law (X-rays, neutrons, electrons)

where λ – wavelength of X-ray beam, d – spacing of reflecting planes, Θ– angle of incidence and reflection, n – order of diffraction (for most of the cases we discuss n=1)

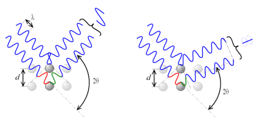
The lattice plane spacing d depends on the crystal structure and indices {hkl} of the planes

$$d_{cubic\_str} = \frac{a}{\sqrt{h^2+k^2+l^2}} \qquad d_{hexagonal\_str} = \frac{a}{\sqrt{\frac{4}{3}\left(h^2+k^2+hk\right)+\frac{l^2a^2}{c^2}}}$$

d – set by the crystal

λ – set by apparatus (constant for a given setup)

can change Θ (theta) or often 2Θ!!!



Kittel, pp.29 - 30

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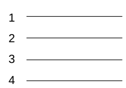
Constructive and destructive interference

X-ray waves scatter ***in phase*** (constructive interference): λ, 2λ, 3λ, …, $n\lambda$ (n – whole number)

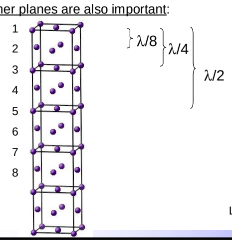
Out of phase (destructive interference): $1/2\lambda$, $3/2\lambda$, $5/2\lambda$, …

What about the other planes?

- if in phase condition holds for plane 1 and 2, it also holds for the plane 3, 4, etc.
- if plane 1 and 2 are out of phase, the 3rd will be in phase will the 1st, … but the 4th will cancel it out



Other planes are also important:



Unless ***constructive interference*** condition met (n – whole number), there is very little intensity at a given angle

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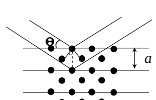
Additional rules

- Consider diffraction from the (100) face of the *fcc* crystal

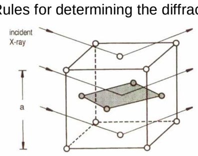


If $2d \sin\Theta = \lambda$ (i.e., n=1)

but there is always another plane at (n=1/2)

$\Rightarrow$ no intensity…

Rules for determining the diffracting {hkl} planes in cubic crystals



Schematic illustration of (100) - (200) annihilation in a fcc lattice.

Lattice	Reflection present	Reflection absent
bcc	(h+k+l)=even	(h+k+l)=odd
fcc	(h,k,l) all odd or even	(h,k,l) not all odd or even

Details of crystal unit cell are important

Different rules for different unit cells

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Possible peaks for cubic structures

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

d_{hkl}	Family of planes	sc	fcc	bcc
a	{100}			

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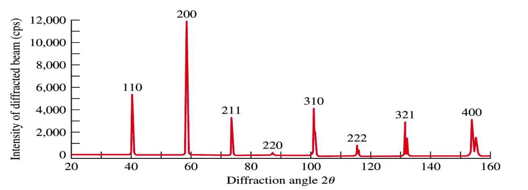
Powder diffraction

- Use polycrystalline sample
  - All possible planes are at angle Θ to beam
  - Only ones satisfying Braggs condition provide diffraction
  - Need to change angle Θ to detect all “Bragg peaks”



Record of the diffraction angles for a **W** (tungsten) sample obtained by the use of a diffractometer with Cu radiation

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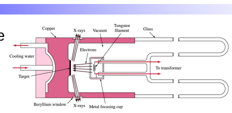
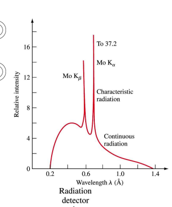
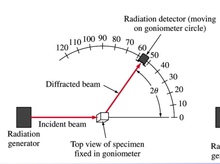
Experimental details (powder diffraction)

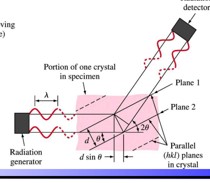
Use polycrystalline sample

- Source
- Collimator (slits)
- Sample holder (need rotation)
- Detector (moves in arc around sample; intensity *vs* 2Θ is recorded)









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