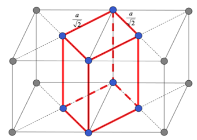
MLL 100
Lec 5
Tue 05.08.2025

Why is End-centred cubic (cS) not in the Bravais list?

Ans 1 (Incorrect reasoning based on unit cell shape)

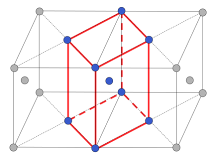


(a) We can select a smaller primitive tetragonal (tP) unit cell.

(b) Primitive tetragonal (tP) is already listed as a Bravais lattice.

(c) So, we do not list end-centred cubic (cS) as a new Bravais lattice

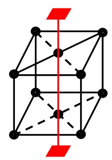
Problem with answer Ans 1



We can select a smaller body-centred tetragonal (tI) unit cell in face-centred cubic (cF) lattice.

But face-centred cubic (cF) is listed as a Bravais lattice.

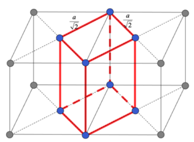
Why is End-centred cubic not in the Bravais list?



Ans 2: Correct symmetry-based reasoning

(a) End-centering destroys the cubic symmetry (Threefold axes along the body diagonals), Therefore it is not a cubic Bravais lattice.

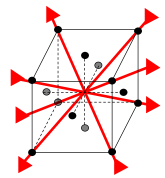
(b) A single 4-fold axis is preserved $\Rightarrow$tetragonal Bravais lattice $(tP$ or $tI)$



(c) We look for tetragonal unit cell and find a primitive tetragonal (tP) unit cell.

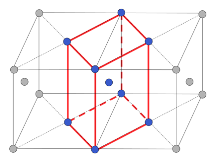
(d) Hence end-centred cubic (cS) is actually tetragonal primitive (tP).

Why CAN'T we call face-centred cubic (cF) as body-centred tetragonal (tI) ?



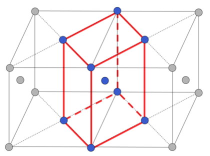
(a) Since all face are centred, four threefold axes are preserved $\Rightarrow$ *Cubic Symmetry*

(b) So the Bravais lattice remains face-centred cubic (cF) even if we can select a body-centred tetragonal unit cell.



(c) Body-centred tetragonal cell is a possible NONCONVENTIONAL cell of the face-centred cubic (cF) lattice.

If Body-centred tetragonal (tI) becomes face-centred cubic (cF) why can't we remove (tI) from the Bravais list?



$tI \rightarrow cF \ only \ for \frac{c}{a} = \sqrt{2}$

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Classification of Symmetry Operations

Does the operation leave a point unmoved?

Yes At least one point remains fixed	No All points move
Point symmetry operation (eg. Rotation)	Space symmetry operation (eg. Translation)

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Symmetry Operations

Rotation	Translation
Reflection	Screw (rot + trans)
Inversion	Glide (ref + trans)
Rotoreflection	
Rotoinversion	NOT FOR MLL100
At least one point remains fixed	No point remains fixed
Point symmetry operation	Space symmetry operation

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Classification of Lattices

Symmetry

Point symmetry (Ignoring translations)
7 types of lattices
7 crystal systems

Space group symmetry (Including translations)
14 types of lattices
14 Bravais lattices

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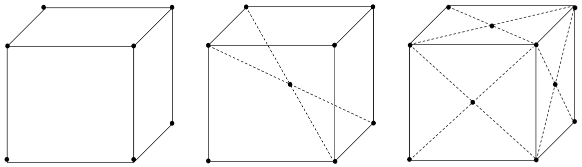
The three cubic Bravais lattices



All have four three-fold axes: Crystal system is Cubic

But they have different translations:
Different Bravais lattices

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Summary of 7 crystal systems and 14 Bravais Lattices

Symmetry and not unit cell shape is the basis for classification of lattices into 7 crystal systems and 14 Bravais Lattices

7 crystal systems: 7 types of symmetry IGNORING translations

14 Bravais lattices: 14 types of symmetry INCLUDING translations

Conventional unit cell shape is based on symmetry.

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Miller Indices of Directions and Planes

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Miller Indices of Directions

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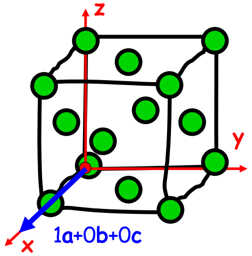
Miller Indices of Directions



1. Choose a point **on the direction** as the origin.

2. Choose a coordinate system with axes parallel to the unit cell edges: **Crystal Coordinate System**

3. Find the coordinates of another point on the direction in terms of **a**, **b** and **c** 1, 0, 0

4. Reduce the coordinates to smallest integers in the same ratio. 1, 0, 0

5. Put in square brackets [100] Usually no commas

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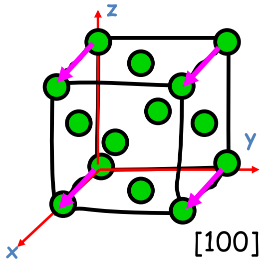
All parallel directions have the same Miller indices



Miller indices of a direction represents only the orientation of the line corresponding to the direction and not its position or sense

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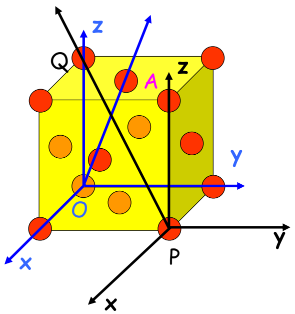
Miller Indices of Directions (Class Exercise)



OA=1/2 **a** *+ 1/2* **b** *+ 1* **c**

1/2, 1/2, 1

[1 1 2]

PQ = -1 **a** -1 **b** + 1 **c**

-1, -1, 1

$[\bar{1}\,\bar{1}\,1]$

-ve steps are shown as bar over the number

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Miller Indices of Directions

Usually, we ignore sense.

$$[uvw] \equiv [\bar{u}\bar{v}\bar{w}]$$

$$[\bar{1}\bar{1}1] \equiv [11\bar{1}]$$

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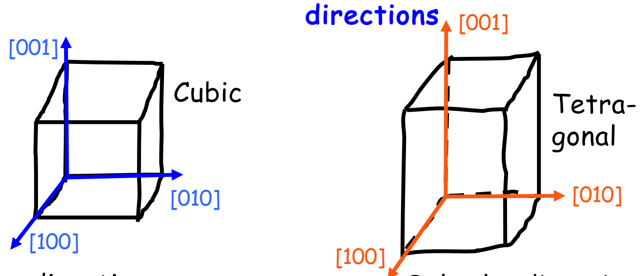
Miller indices of a family of symmetry related directions



The directions $[100], [010] and [001]$ can be mapped into each other by the cubic symmetry

Only the directions $[100], [010]$ can be mapped into each other by the tetragonal symmetry

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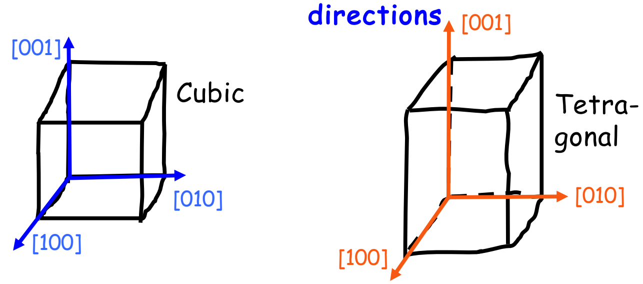
Miller indices of a family of symmetry related directions



$$\langle 100\rangle_{Cubic} = \{[100], [010], [001], [\bar{1}00], [0\bar{1}0], [00\bar{1}]\}$$

$$\langle 100\rangle_{tetragonal} = \{[100], [010], [\bar{1}00], [0\bar{1}0]]\}$$

$$\langle 001\rangle_{tetragonal} = \{[001], [00\bar{1}]\}$$

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Miller indices of a family of symmetry related directions

$$\langle uvw\rangle$$

$[uvw]$ and all other directions related to $[uvw]$ by the symmetry of the crystal

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Miller Indices for planes

Crystallographic Coordinate system

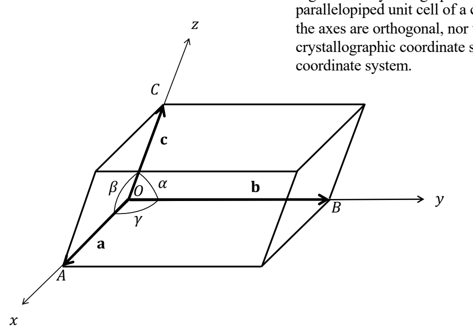
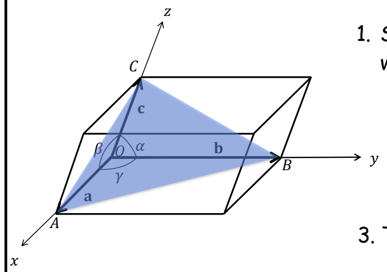


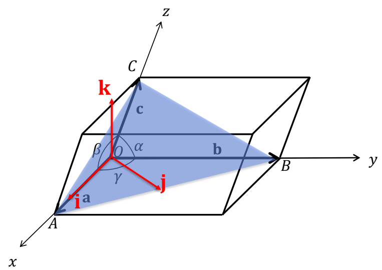
Figure 3.1 Crystallographic coordinate system attached to the parallelopiped unit cell of a crystal. Note that in general neither the axes are orthogonal, nor the basis vectors are unit vectors. A crystallographic coordinate system is different from a Cartesian coordinate system.

Miller Indices of a plane

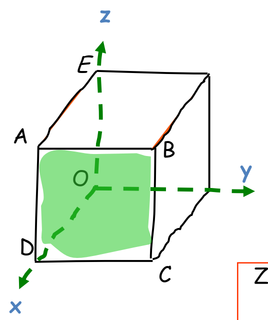


1. Select a crystallographic coordinate system with **ORIGIN NOT ON THE PLANE**
2. Find INTERCEPTS along axes in terms of RESPECTIVE LATTICE PARAMETERS 1 1 1
3. Take the RECIPROCALS 1 1 1
4. Convert to smallest integers in the same ratio 1 1 1
5. Enclose in PARENTHESIS (111)

Miller Indices of a plane



Miller Indices of a plane



Plane	ABCD
origin	O
intercepts	1 ∞ ∞
reciprocals	1 0 0
Small integers	1 0 0
Miller Indices	(1 0 0)

Zero represents that the plane is parallel to the corresponding axis

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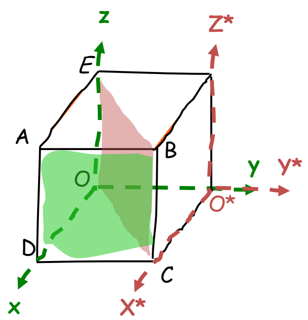
Miller Indices of a plane



Plane	OCBE
origin	O*
intercepts	1 -1 ∞
reciprocals	1 -1 0
Miller Indices	$(1\,\bar{1}\,0)$

Bar represents a negative intercept

Model Answer to exam question:
Plane (ABCD) is (100) with O as origin
Plane (OCBE) is (110) with O* as origin.

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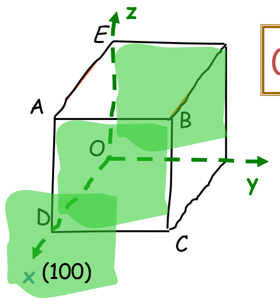
Miller indices of a plane specifies only its orientation in space not its position

All parallel planes have the same Miller Indices

$(h\,k\,l) \parallel (\bar{h}\,\bar{k}\,\bar{l})$



$(100) \parallel (\bar{1}00)$

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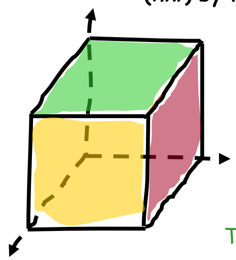
Miller indices of a family of symmetry related planes

{*hkl*} = (*hkl*) and all other planes related to (*hkl*) by the symmetry of the crystal



All the faces of the cube are equivalent to each other by symmetry

Front & back faces: (100), $(\bar{1}00)$
Left and right faces: (010), $(0\bar{1}0)$
Top and bottom faces: (001) $(00\bar{1})$

$\{100\}_{cubic} = (100), (010), (001), (\bar{1}00), (0\bar{1}0), (00\bar{1})$

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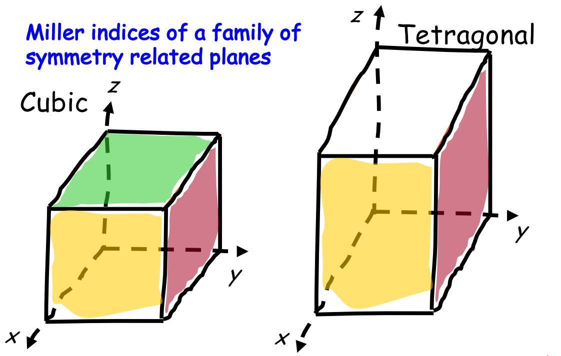
Miller indices of a family of symmetry related planes



$\{100\}_{cubic} = (100), (010), (001), (\bar{1}00), (0\bar{1}0), (00\bar{1})$

$\{100\}_{tetragonal} = (100), (010), \cancel{(001)}, (\bar{1}00), (0\bar{1}0), \cancel{(00\bar{1})}$

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Miller Indices Brackets

$[uvw]$ *Single direction of parallel directions*

$\langle uvw \rangle$ *Direction $[uvw]$ and all directions related to it by symmetry of the crystal*

(hkl) *Single Plane (hkl) or a set of parallel planes*

$\{hkl\}$ *Plane (hkl) and all planes related to it by symmetry of the crystal*

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Some IMPORTANT Results

Weiss zone law

Condition for a direction [*uvw*] to be parallel to a plane or lie in the plane (*hkl*):

$$\boxed{h\,u + k\,v + l\,w = 0}$$

True for ALL crystal systems. Proof left as an exercise.

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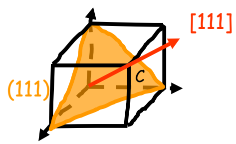
CUBIC CRYSTALS

$\boxed{[hkl] \perp (hkl)}$



For cubic crystals the directions and planes with the same Miller indices are always perpendicular.

Proof left as an exercise.

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Try problems from
Chapter 3 of V, Raghavan, Introduction to materials Science and Engineering, Fifth Edition

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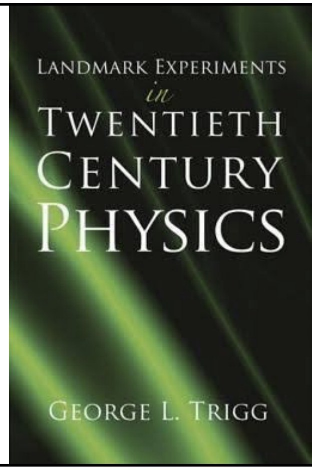

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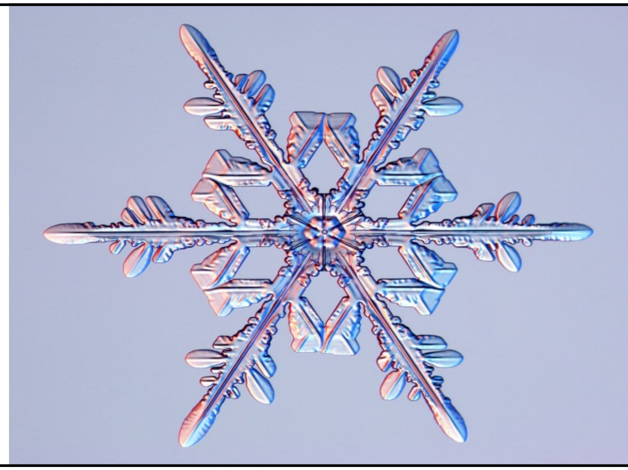

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Courtsey: Wtodi, www.flickr.com.

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By H. Raab (User:Vesta) (Own work), Wikipedia

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Solid

Crystalline

Amorphous

Crystal (Definition 1):

Crystals are solids with regular external shape as a result of natural growth

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Question 1:

Why crystal have regular external shapes?

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Johannes Kepler

Six-cornered snow flake

A new year gift to his patron in 1611

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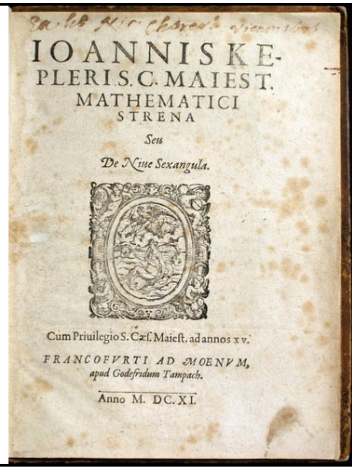
IOANNIS KE-
PLERI S.C. MAIEST.
MATHEMATICI
STRENA
Seu
De Niue Sexangula.

Cum Priuilegio S. Cæs. Maiest. ad annos xv.

FRANCOFVRTI AD MOENVM,
apud Godefridum Tampach.

Anno M. DC. XI.

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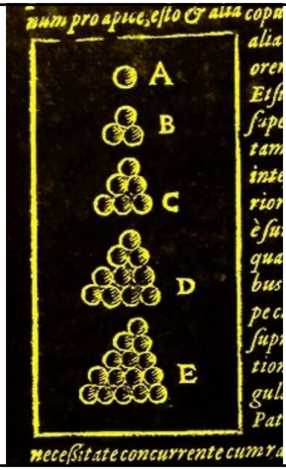

1611

Kepler’s de Nive Sexangula

“A New Year Gift or Six-Cornered Snowflake”

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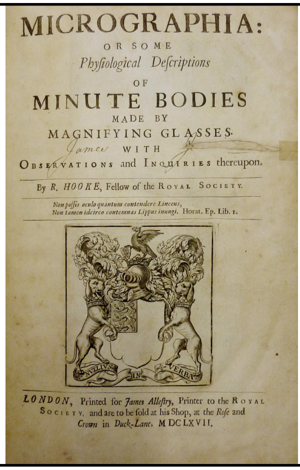
Robert Hooke:

44

1667


MICROGRAPHIA:
OR SOME
Physiological Descriptions
OF
MINUTE BODIES
MADE BY
MAGNIFYING GLASSES.
WITH
OBSERVATIONS and INQUIRIES thereupon.

By *R. HOOKE*, Fellow of the ROYAL SOCIETY.

Non possis oculo quantum contendere Linceus,
Non tamen idcirco contemnas Lippus inungi. Horat. Ep. Lib. 1.

NULLIUS IN VERBA

LONDON, Printed for *James Allestry*, Printer to the ROYAL SOCIETY, and are to be sold at his Shop, at the *Rose* and *Crown* in *Duck-Lane*. MDCLXVII.

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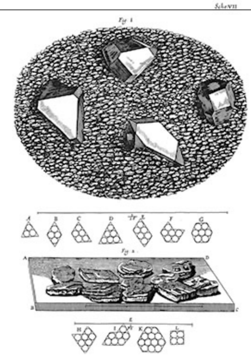

Hooke's Micrographia, 1665

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Postulate 1:

Regular external shapes of the crystal is due to regular internal arrangement of their building blocks.

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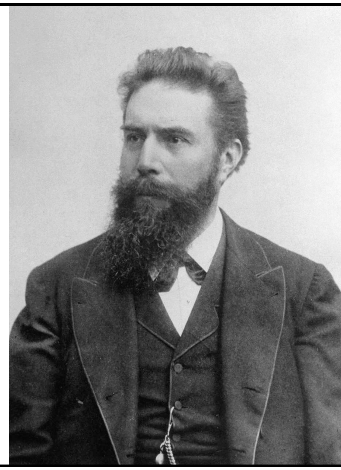
1895

Wilhelm Röntgen
Discovered x-rays

First Nobel Prize in physics: 1901



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First x-ray picture
November 1895

Hand of Roentgen's wife

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Question2:
Are x-rays waves
or particles?

X stands for the unknown

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Laue's Postulate

If crystals are periodic arrangement of atoms

And

If x-rays are waves

Then

Crystals should act as a 3D diffraction grating for x-rays

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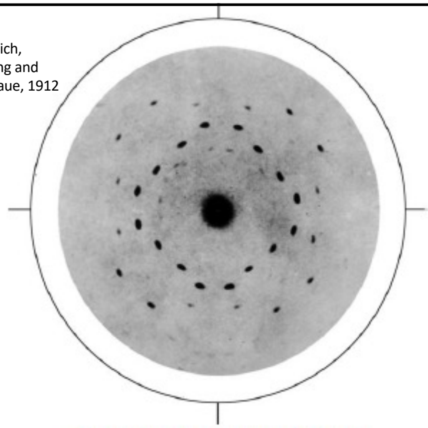
W. Friedrich,
P. Knipping and
M. von Laue, 1912



X-ray photograph of zinc blende

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Two **GREAT** results from a single experiment:

1. X-rays are waves

2. Crystals are periodic arrangement of atoms

One of the greatest scientific discoveries of twentieth century

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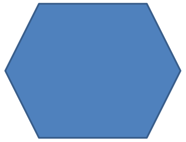
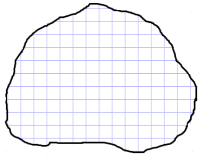
Crystallographic Revolution 1912

Crystal (Definition 1):
Crystals are solids with regular external shape as a result of natural growth



Crystal (Definition 2):
Crystals are solids with periodic arrangement of atoms



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Some crystal structures

Crystal	Lattice	Motif	Lattice parameter
Cu	FCC	Cu 000	a=3.61 Å
Zn	Simple Hex	Zn 000, Zn 1/3, 2/3, 1/2	a=2.66 c=4.95

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Q1: How do we determine the crystal structure?

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Crystallographic Revolution

X-ray diffraction as an experimental tool to explore the internal structure of crystals

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J.J Thomson got Nobel Prize in 1906 for showing that electrons are particles

His son GP Thomson got Nobel Prize in 1937 for showing that electrons are waves.

Which is the only father-son team to win a Nobel prize? For what?

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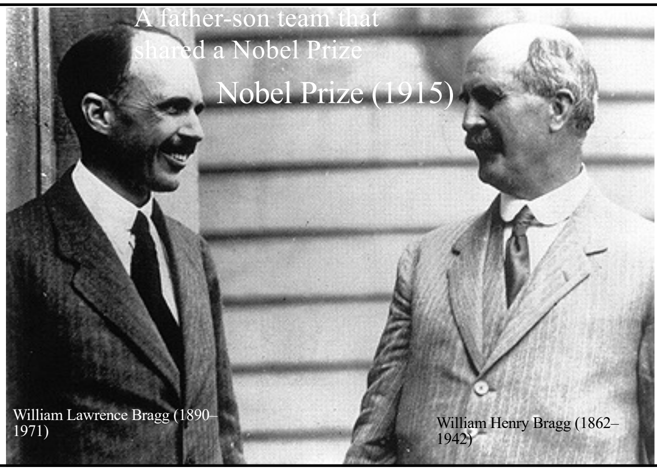

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X-Ray Diffraction = Peak Positions + Peak Intensities

↕ ↕ ↕

Crystal Structure = Lattice + Motif: Atom Positions

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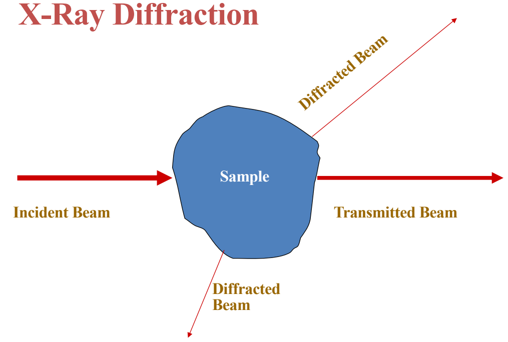
X-Ray Diffraction



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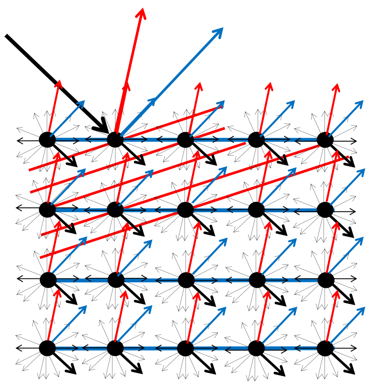

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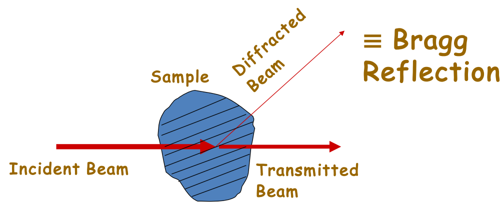
X-Ray Diffraction = Reflection



Braggs Law (Part 1): For every diffracted beam there exists a set of crystal lattice planes such that the diffracted beam appears to be specularly reflected from this set of planes.

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X-Ray Diffraction

Braggs' recipe for Nobel prize?

Call the diffraction a reflection!!!

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"The important thing in science is not so much to obtain new facts as to discover new ways of thinking about them".

W.L. Bragg

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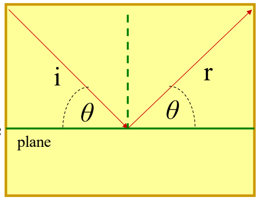
X-Ray Diffraction

Braggs Law (Part 1): the diffracted beam appears to be **specularly** reflected from a set of crystal lattice planes.

Specular reflection:
Angle of incidence
=Angle of reflection
(both measured from the plane and not from the normal)



The incident beam, the reflected beam and the plane normal lie in one plane

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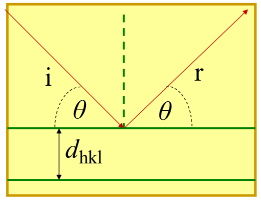
X-Ray Diffraction



Bragg's law (Part 2):

$$n\lambda = 2d_{hkl}\sin\theta$$

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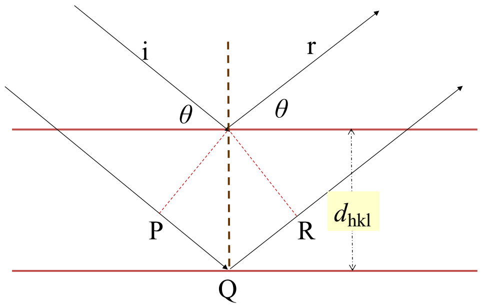

Path Difference =PQ+QR $= 2d_{hkl}\sin\theta$

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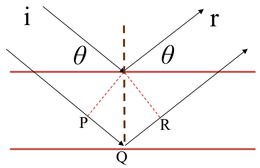

Path Difference =PQ+QR $= 2d_{hkl}\sin\theta$

Constructive inteference

$$n\lambda = 2d_{hkl}\sin\theta$$

Bragg's law

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d_{hkl}?

Interplanar spacing

Between parallel planes

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Family of parallel (hkl) planes and interplanar spacing d_{hkl}

(hkl) plane

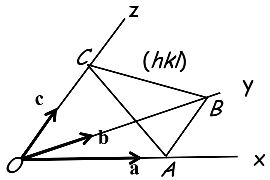
Relative Intercepts: $\frac{1}{h};\frac{1}{k};\frac{1}{l}$

Actual Intercepts: $\frac{a}{h};\frac{b}{k};\frac{c}{l}$

$OA = \frac{a}{h}$

$OB = \frac{b}{k}$

$OC = \frac{c}{l}$



Parallel (hkl) planes with intercepts:

$\frac{na}{h};\frac{nb}{k};\frac{nc}{l}$ with $n = \cdots -2, -1, 0, +1, +2, \ldots$

d_{hkl} = spacing between successive (hkl) planes

= spacing between a parallel plane through origin $(n = 0)$ and first plane away from origin

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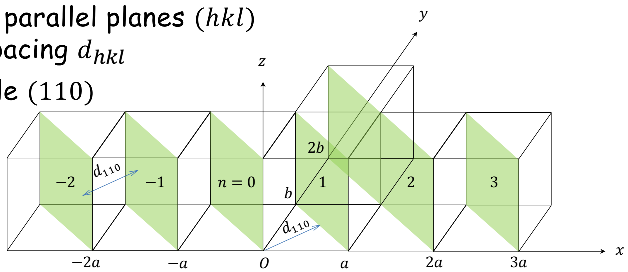
Set of parallel planes (hkl) with spacing d_{hkl}

Example (110)



For any (hkl) draw a first plane with intercepts $\frac{a}{h},\frac{b}{k},\frac{c}{l}$. Call this the first plane plane $n = 1$

Draw a parallel plane through the origin. This is $n = 0$ plane.

Distance between these two planes, or equivalently distance of $n = 1$ from the origin, is defined as d_{hkl}

Draw other equidistant planes with spacing d_{hkl} and intercepts given by $\frac{na}{h},\frac{nb}{k},\frac{nc}{l}$

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Miller Indices of planes vs. indices of reflections

In Miller indices we take $(nh\,nk\,nl) \equiv (hkl)$

But in context of diffraction $nh\,nk\,nl \neq hkl$

$nh\,nk\,nl$ is the index of nth order reflection whereas hkl is the index of the $1st$ order reflection from the (hkl) plane

To distinguish between the index of reflection, which allows common factors and Miller indices of planes where we cancel the common factors we will write the **indices of reflections without parentheses**, whereas for Miller indices of planes we use parentheses.

Thus 111 and 222 are 1st and 2nd order reflections from (111) plane.

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Relation between $(nh\ nk\ nl)$ and (hkl)

$$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

$$\frac{1}{d_{nh\,nk\,nl}^2} = \frac{n^2h^2}{a^2} + \frac{n^2k^2}{b^2} + \frac{n^2l^2}{c^2} = n^2\left(\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right) = \frac{n^2}{d_{hkl}^2}$$

$$d_{nh\,nk\,nl} = \frac{d_{hkl}}{n}$$

d_{hkl} is a homogeneous function of degree -1

$$d_{200} = \frac{d_{100}}{2} \qquad d_{333} = \frac{d_{111}}{3}$$

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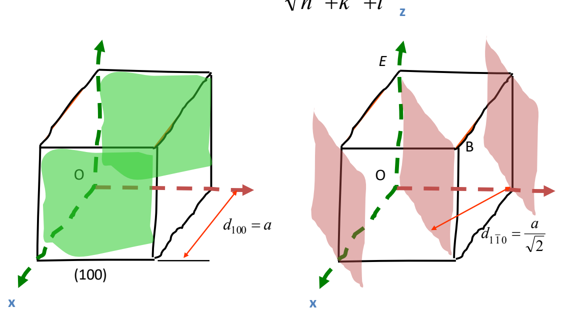
$\boxed{d_{hkl}}$

Proof as an exercise

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



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$$n\lambda = 2d_{hkl}\sin\theta$$

n

Order of diffraction

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$n = 1$

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Two equivalent ways of stating Bragg's Law

$$\boxed{n\lambda = 2d_{hkl}\sin\theta}$$ Physicist's Form

$$\Rightarrow \lambda = 2\frac{d_{hkl}}{n}\sin\theta$$

$$d_{nh,nk,nl} = \frac{a}{\sqrt{(nh)^2+(nk)^2+(nl)^2}} = \frac{d_{hkl}}{n}$$

$$\boxed{\Rightarrow \lambda = 2d_{nh\,nk\,nl}\sin\theta}$$ Crystallographer's Form

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Two equivalent ways of stating Bragg's Law

$$\boxed{n\lambda = 2d_{hkl}\sin\theta} \quad \boxed{\Rightarrow \lambda = 2d_{nh\,nk\,nl}\sin\theta}$$

n^{th} order reflection from (*hkl*) plane

1^{st} order reflection from (*nh nk nl*) plane

e.g. a 2^{nd} order reflection from (111) plane can be described as 1^{st} order reflection from (222) plane

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In X-ray Diffraction (*hkl*) can have common factors.

The common factor represents the order of diffraction.

(*nh nk nl*) diffraction is nth order diffraction from (*hkl*) plane

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X-rays
Characteristic Radiation, K_α

Target	*Wavelength, Å*
Mo	0.71
Cu	1.54
Co	1.79
Fe	1.94
Cr	2.29

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Powder Method

λ is fixed (K_α radiation)

θ is variable – specimen consists of millions of powder particles – each being a crystallite and these are randomly oriented in space – amounting to the rotation of a crystal about all possible axes

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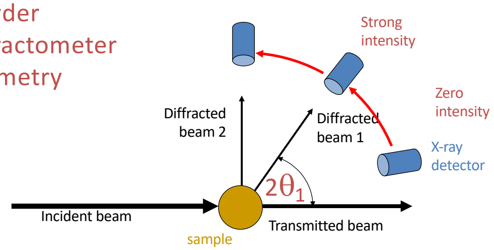
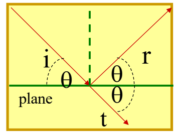
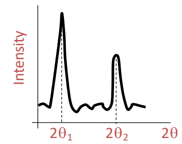
Powder diffractometer geometry







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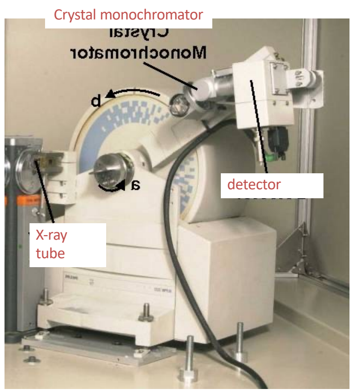

X-ray powder diffractometer

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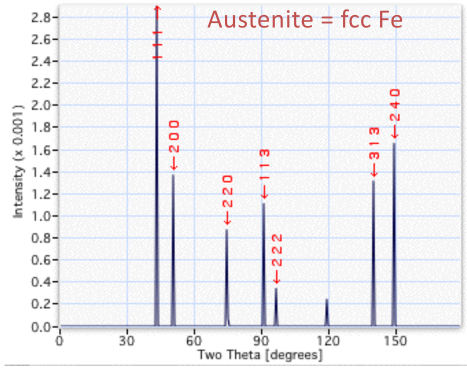
The diffraction pattern of austenite



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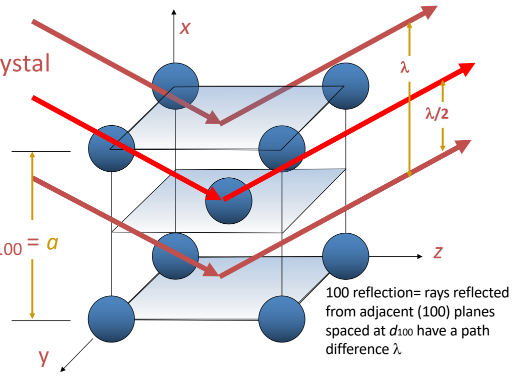
Bcc crystal



No 100 reflection for bcc

No bcc reflection for *h+k+l*=odd

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Extinction Rules: Table 3.3 Raghavan

Bravais Lattice	Allowed Reflections
SC	All
BCC	(h + k + l) even
FCC	h, k and l unmixed
DC	h, k and l are all odd *Or* *if* all are even *then* *(h + k + l) divisible by 4*

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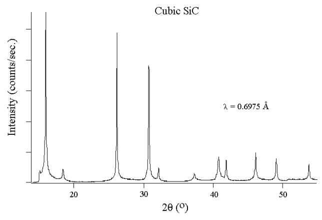
Diffraction analysis of cubic crystals

Bragg's Law:

$$\boxed{\lambda = 2d_{hkl}\sin\theta} \quad (1)$$

Cubic crystals

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



(2) in (1) => $\sin^2\theta = \frac{\lambda^2}{4a^2}(h^2+k^2+l^2)$

constant

$$\sin^2\theta \propto (h^2+k^2+l^2)$$

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