

TEQIP WORKSHOP ON HIGH RESOLUTION X-RAY  
AND ELECTRON DIFFRACTION, FEB 01, 2016, IIT-K.

# BASIC CRYSTALLOGRAPHY

Rajesh Prasad

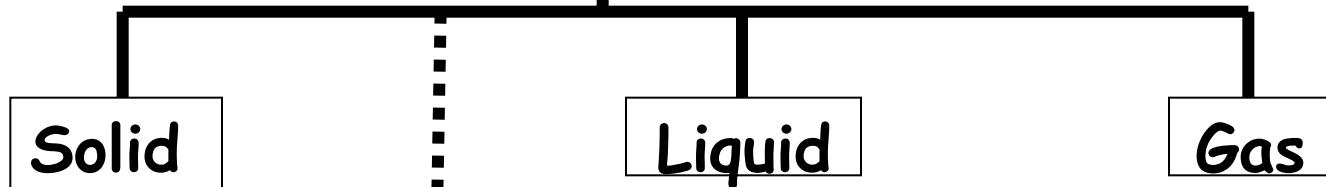
Department of Applied Mechanics  
Indian Institute of Technology  
New Delhi 110016

[rajesh@am.iitd.ac.in](mailto:rajesh@am.iitd.ac.in)

# Applied Mechanics, IIT-D

- Solid Mechanics
- Fluid Mechanics
- Materials Science
  - Rajesh Prasad: Physical Metallurgy
    - Metal Foam (K.L.A. Khan, Gunjit Kumar)
    - Friction Stir Welding (Md.Z.K. Yusufzai, Deepti Goel, Ratnesh)
    - MD of Polymer Nanocomposite (Apoorva Mandal)
    - Equal Channel Angular Pressing (S. Giribaskar at IIT-K)
  - Jayant Jain: Physical Metallurgy
  - Anamika Prasad: Biomedical materials
  - Ashish Garg: Electronic materials

# Matter



*Liquid  
crystal*



**Crystalline**

**Amorphous**

*Quasicrystals*

Nobel Prize 2011

# Lattice?

A 3D translationally periodic arrangement of points in space is called a lattice.

# Classification of Lattices

Lattices

|

7 crystal  
systems

|

14 Bravais  
Lattices

# 7 Crystal Systems and 14 Bravais Lattices

Crystal System	Bravais Lattices			
1. Cubic	P	I	F	
2. Tetragonal	P	I		
3. Orthorhombic	P	I	F	C
4. Hexagonal	P			
5. Trigonal	P			
6. Monoclinic	P			C
7. Triclinic	P			

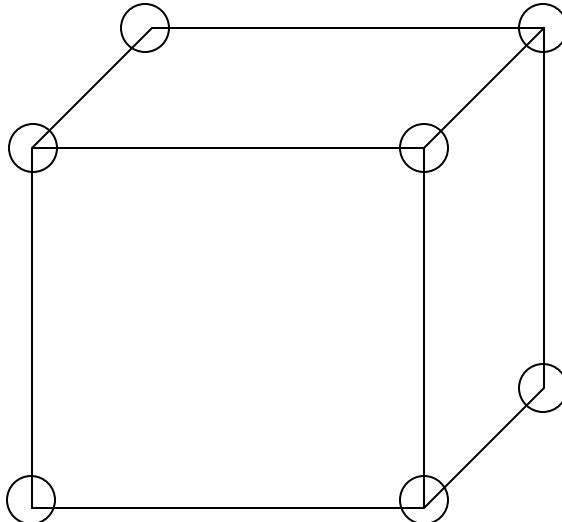
P: Simple; I: body-centred;

F: Face-centred; C: End-centred

# The three cubic Bravais lattices

Crystal system

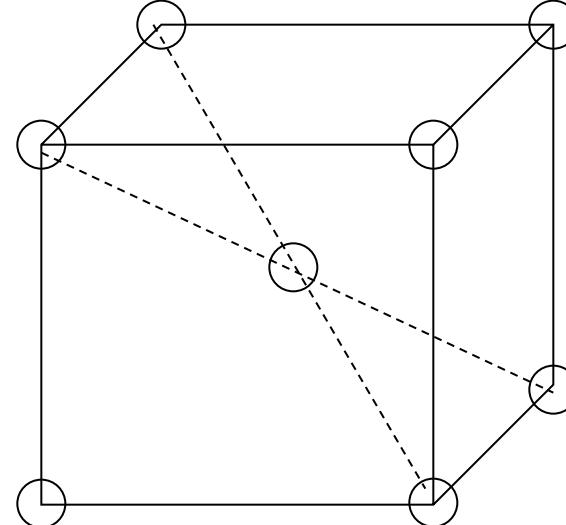
1. Cubic



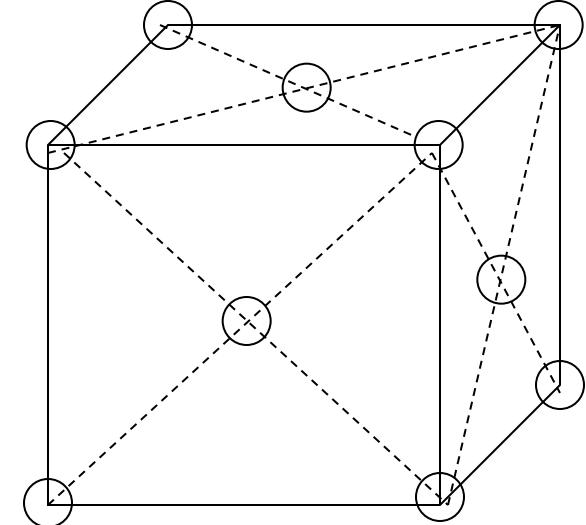
Simple cubic  
Primitive cubic  
Cubic P

Bravais lattices

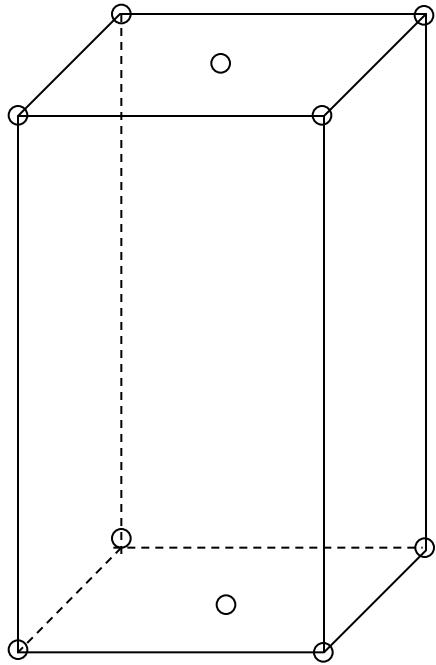
P I F



Body-centred cubic  
Cubic I



Face-centred cubic  
Cubic F



Orthorhombic C  
End-centred orthorhombic  
Base-centred orthorhombic

# Cubic Crystals?

$a=b=c; \alpha=\beta=\gamma=90^\circ$

# 7 crystal Systems

## Unit Cell Shape

1.  $a=b=c, \alpha=\beta=\gamma=90^\circ$

2.  $a=b \neq c, \alpha=\beta=\gamma=90^\circ$

3.  $a \neq b \neq c, \alpha=\beta=\gamma=90^\circ$

4.  $a=b \neq c, \alpha=\beta=90^\circ, \gamma=120^\circ$

5.  $a=b=c, \alpha=\beta=\gamma \neq 90^\circ$

6.  $a \neq b \neq c, \alpha=\beta=90^\circ \neq \gamma$

7.  $a=b \neq c, \alpha \neq \beta \neq \gamma$

## Crystal System

Cubic

Tetragonal

Orthorhombic

Hexagonal

Rhombohedral  
OR Trigonal

Monoclinic

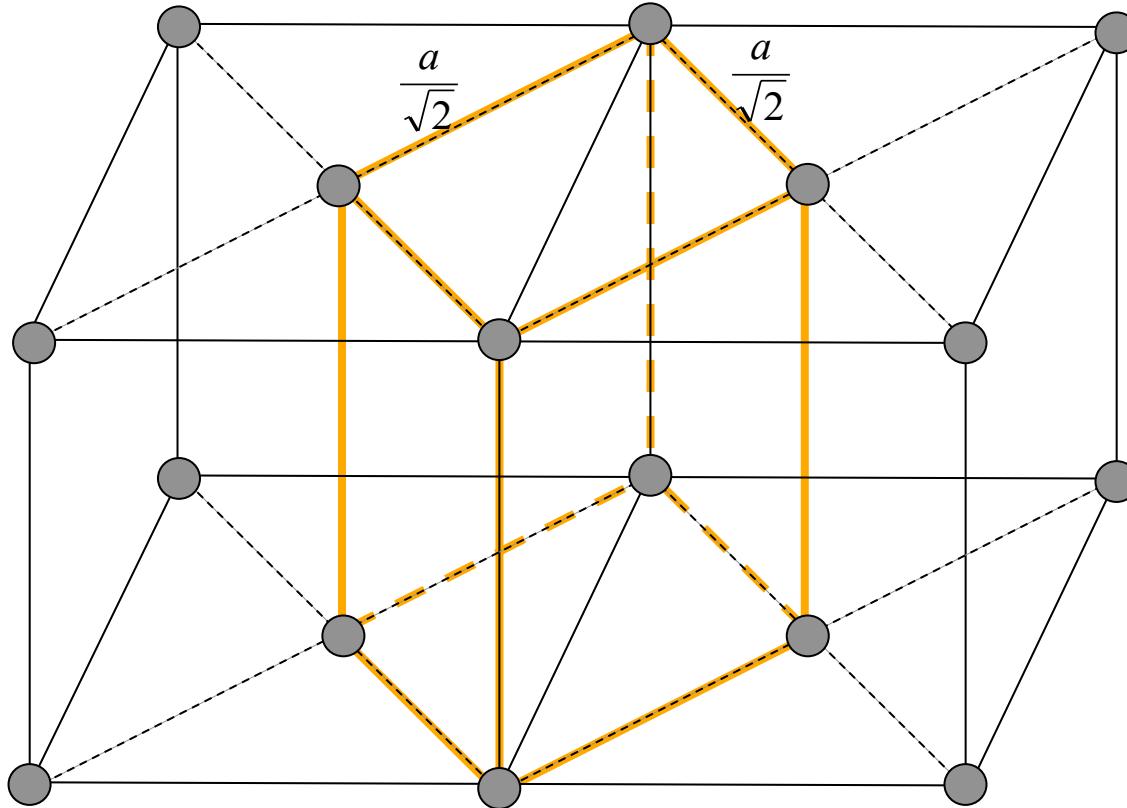
Triclinic

# Why half the boxes are empty?

Crystal System	Bravais Lattices			
1. Cubic	P	I	F	?
2. Tetragonal	P	I		
3. Orthorhombic	P	I	F	C
4. Hexagonal	P			
5. Trigonal	P			
6. Monoclinic	P			C
7. Triclinic	P			

E.g. Why cubic C is absent?

# End-centred cubic not in the Bravais list ?

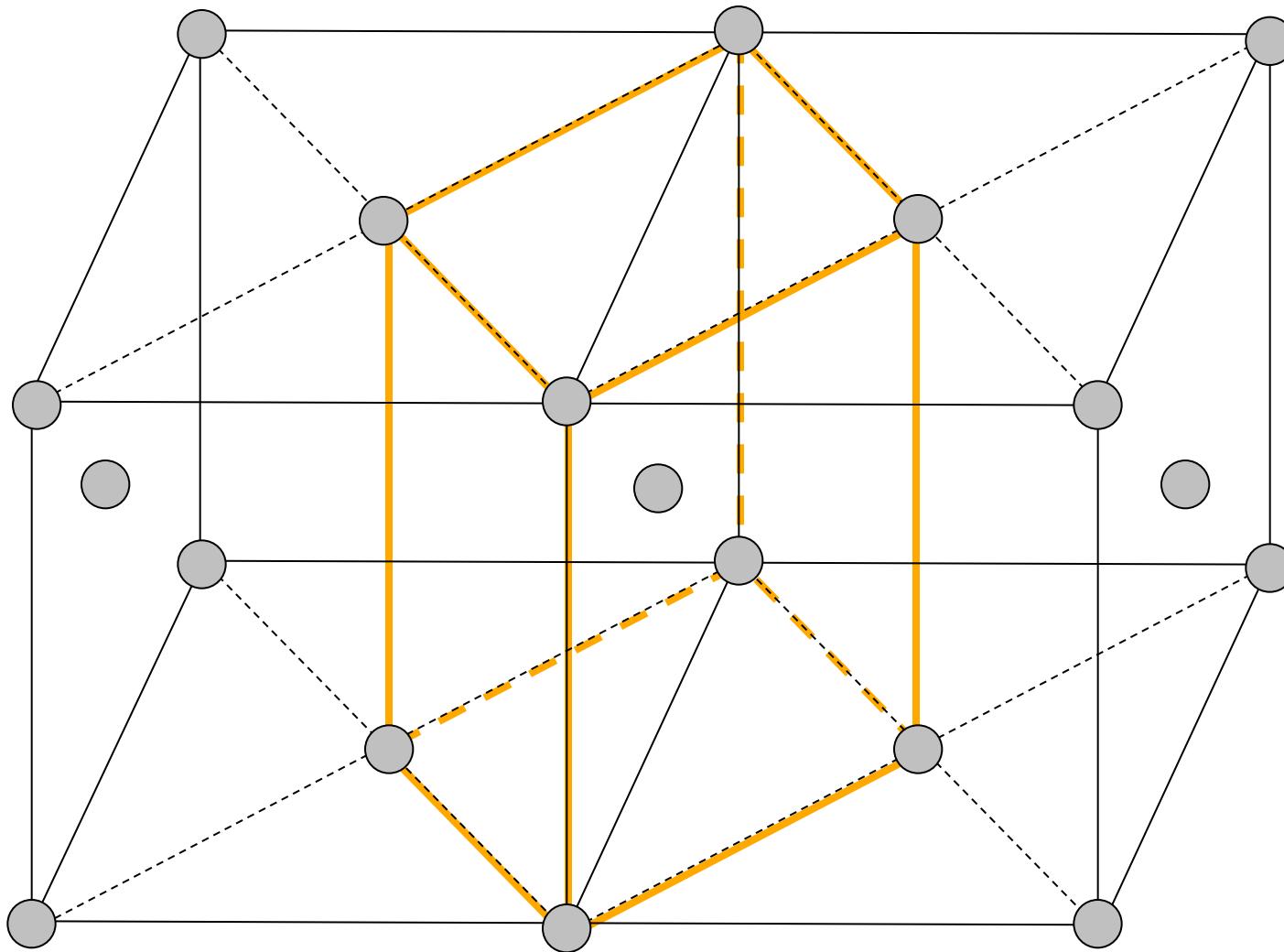


**End-centred cubic = Simple Tetragonal**

# 14 Bravais lattices divided into seven crystal systems

Crystal system	Bravais lattices			
1. Cubic	P	I	F	C
2. Tetragonal	P	I		
3. Orthorhombic	P	I	F	C
4. Hexagonal	P			
5. Trigonal	P			
6. Monoclinic	P			C
7. Triclinic	P			

Now apply the same procedure to the FCC lattice



Cubic F = Tetragonal I ???

# 14 Bravais lattices divided into seven crystal systems

Crystal system

1. Cubic

2. Tetragonal

3. Orthorhombic

4. Hexagonal

5. Trigonal

6. Monoclinic

7. Triclinic

Bravais lattices

P

I

F

C

P

I

F

C

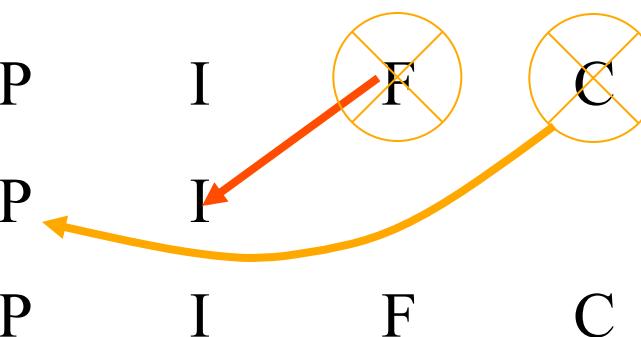
P

P

P

P

C



# History:

**ML Frankenheim**

1801-1869

1835: **X** lattices

1856: 14 lattices

Couldn't  
find his  
photo on  
the net

Auguste Bravais

1811-1863

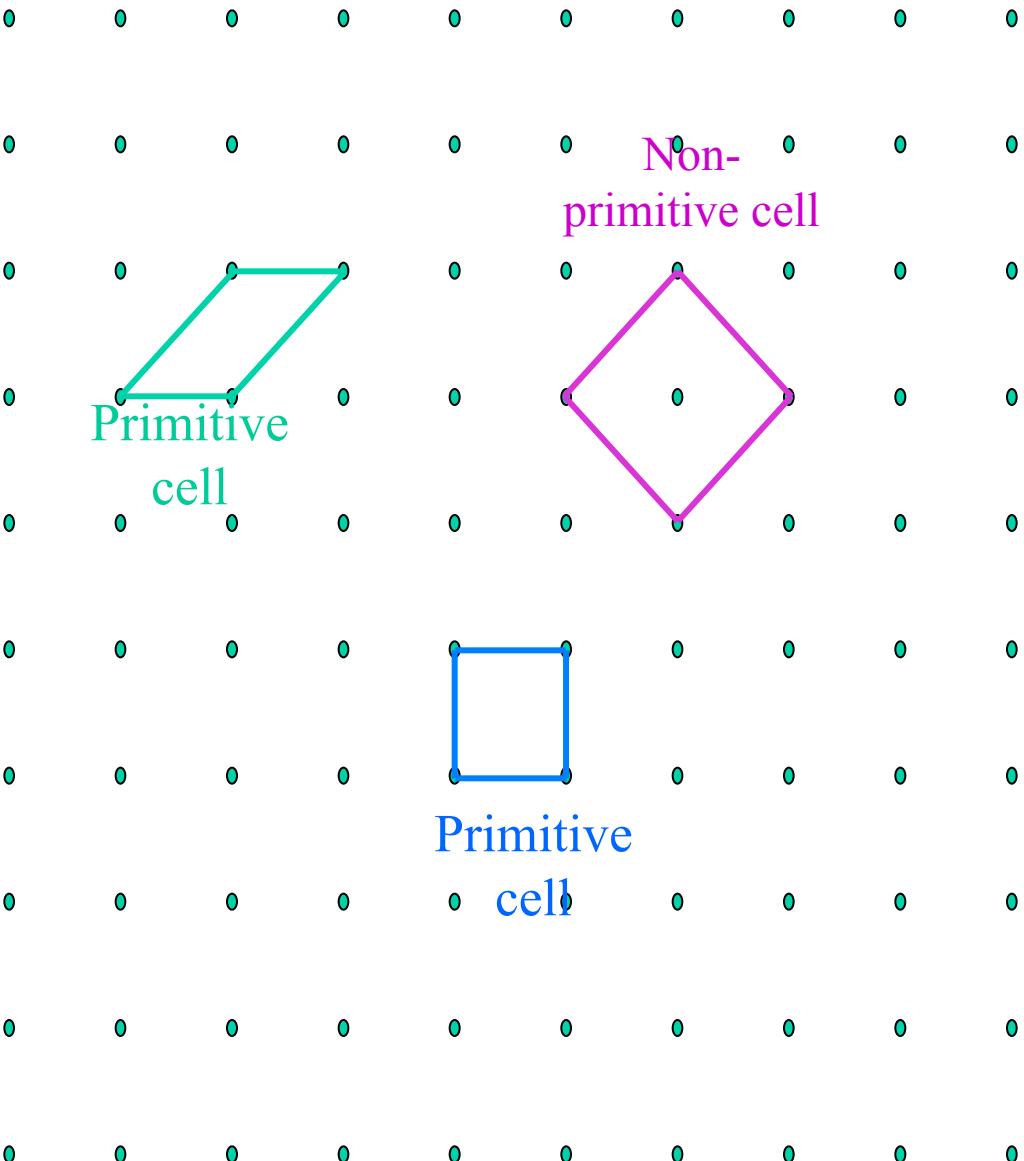
1850: 14 lattices

**KANPUR**

1<sup>ST</sup> FEB. 2016:  
13 lattices !!!



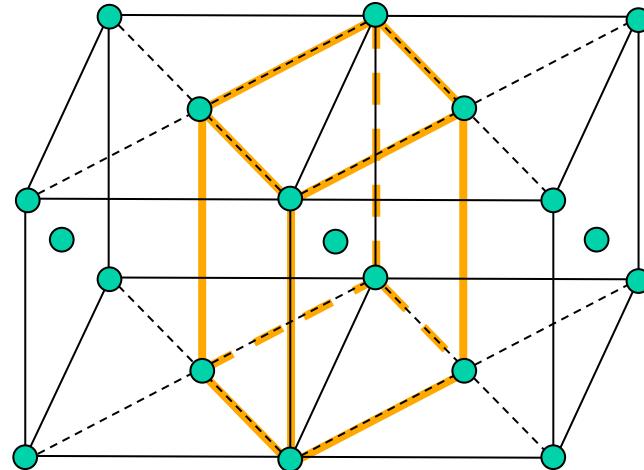
# UNIT CELLS OF A LATTICE



A unit cell of a lattice is **NOT** unique.

Unit cell shape **CANNOT** be the basis for classification of Lattices

Why can't the Face-Centred Cubic lattice (Cubic F) be considered as a Body-Centred Tetragonal lattice (Tetragonal I) ?



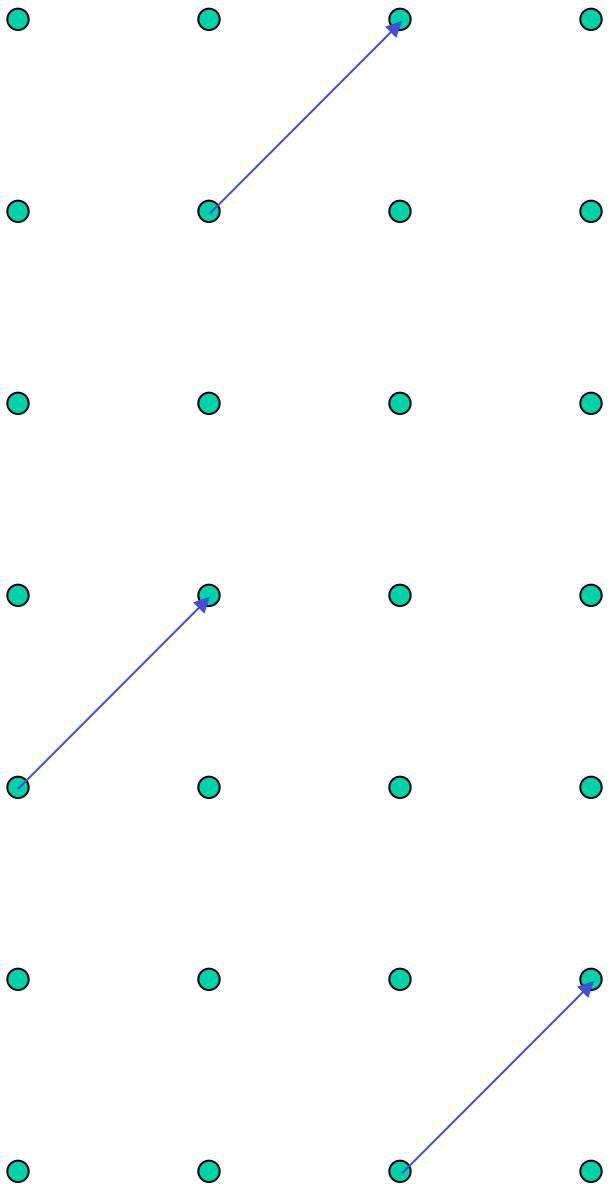
What is the basis for  
classification of lattices  
into  
7 crystal systems  
and  
14 Bravais lattices?

Lattices are  
classified on the  
basis of their  
symmetry

# Symmetry?

If an object is brought into self-coincidence after some operation it said to possess symmetry with respect to that operation.

# Translational symmetry



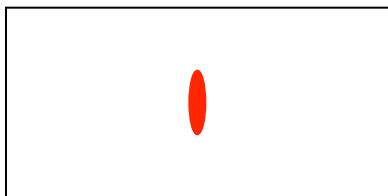
Lattices also have  
**translational**  
**symmetry**

In fact this is the  
defining symmetry of  
a lattice

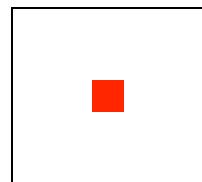
# Rotation Axis

If an object come into self-coincidence through smallest non-zero rotation angle of  $\theta$  then it is said to have an n-fold rotation axis where

$$n = \frac{360^\circ}{\theta}$$



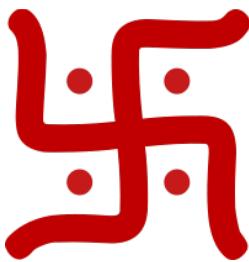
$\theta=180^\circ$     n=2    2-fold rotation axis



$\theta=90^\circ$     n=4    4-fold rotation axis

# Examples of Rotational Symmetry

Z



Angles:

180°    120°    90°    72°    60°    45°

Fold:

2    3    4    5    6    8

Graphic symbols



# Crystallographic Restriction

5-fold symmetry or Pentagonal symmetry is not possible for Periodic Tilings

Symmetries higher than 6-fold also not possible

Only possible rotational symmetries for lattices



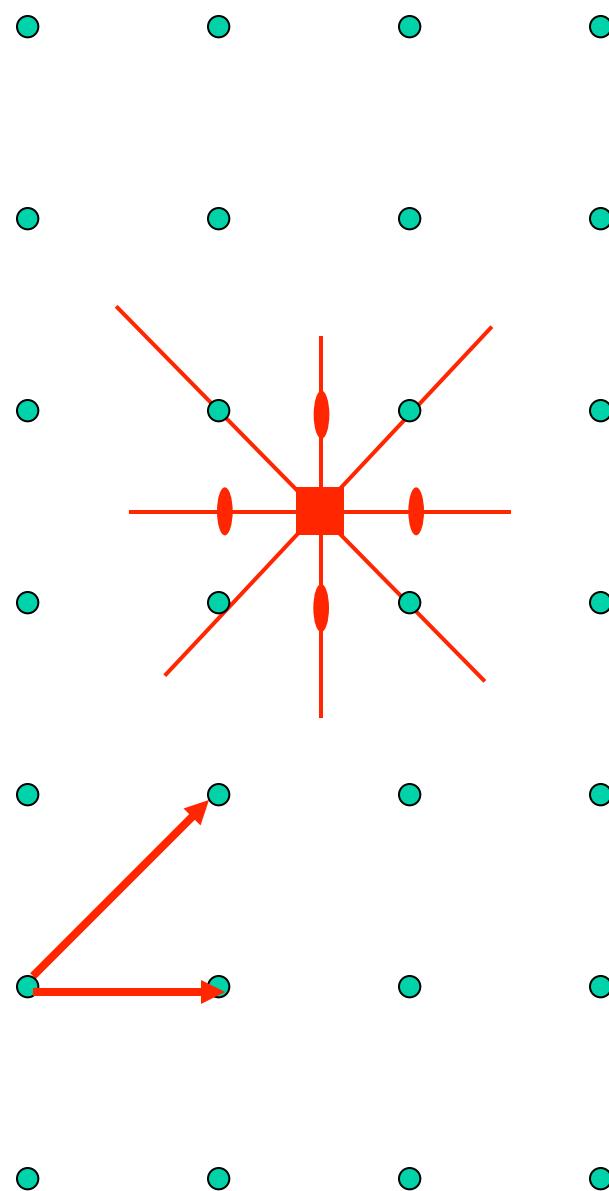
# Symmetry of lattices

Lattices have

Translational symmetry

Rotational symmetry

Reflection symmetry



# Point Group and Space Group

The group of all symmetry elements of a crystal except translations (e.g. rotation, reflection etc.) is called its **POINT GROUP**.

The complete group of all symmetry elements including translations of a crystal is called its **SPACE GROUP**

# Classification of Lattices

## Crystal systems and Bravais Lattices

Based on the point group symmetry alone (i.e. excluding translational symmetry)

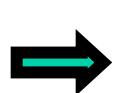
- ⇒ 7 types of lattices
- ⇒ 7 crystal systems

Based on the space group symmetry, i.e., rotational, reflection and translational symmetry

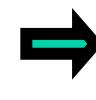
- ⇒ 14 types of lattices
- ⇒ 14 Bravais lattices

# 7 crystal Systems

Defining symmetry



Crystal system



Conventional unit cell

4 or

Cubic

$a=b=c, \alpha=\beta=\gamma=90^\circ$

only 1 or

Tetragonal

$a=b\neq c, \alpha=\beta=\gamma=90^\circ$

3 or

Orthorhombic

$a\neq b\neq c, \alpha=\beta=\gamma=90^\circ$

1 or

Hexagonal

$a=b\neq c, \alpha=\beta=90^\circ, \gamma=120^\circ$

only 1 or

Rhombohedral

$a=b=c, \alpha=\beta=\gamma\neq90^\circ$

only 1 or

Monoclinic

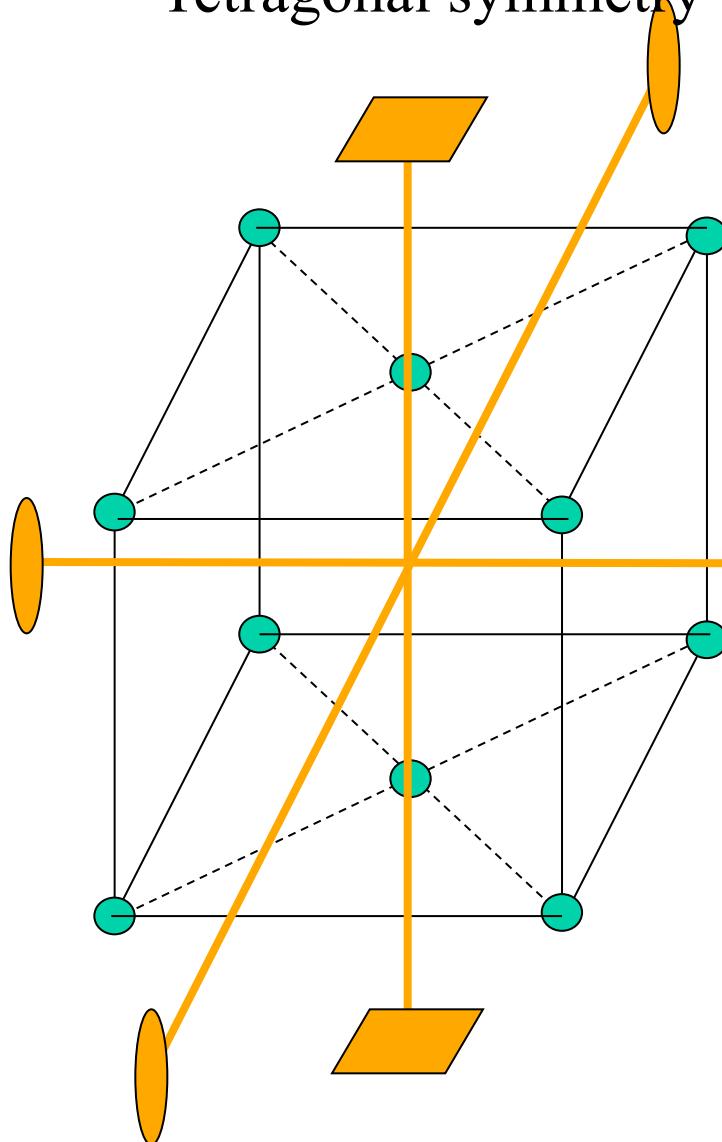
$a\neq b\neq c, \alpha=\beta=90^\circ\neq\gamma$

None or i

Triclinic

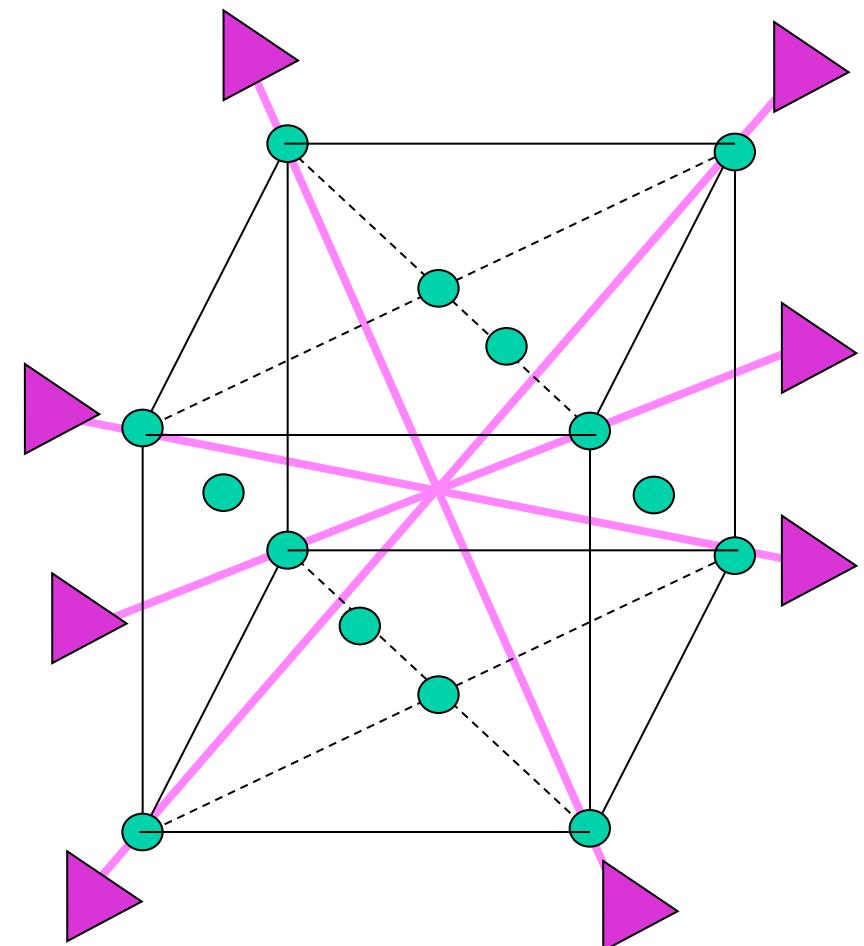
$a\neq b\neq c, \alpha\neq\beta\neq\gamma$

Tetragonal symmetry



Cubic C = Tetragonal P

Cubic symmetry

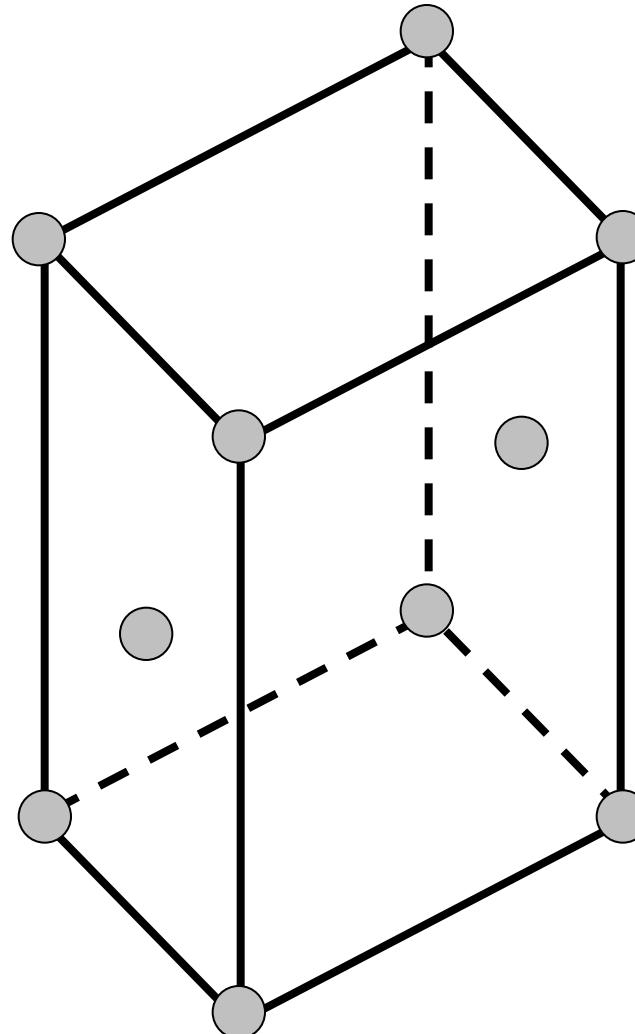


Cubic F  $\neq$  Tetragonal I

$$a=b \neq c, \alpha=\beta=\gamma=90^\circ$$

A tetragonal unit cell with two opposite rectangular faces centred.

Bravais Lattice?



# Crystal ?

A 3D translationally periodic arrangement of atoms in space is called a crystal.

# Crystal vs. Lattice

Crystal

A 3D  
translationally  
periodic  
arrangement  
of atoms

Lattice

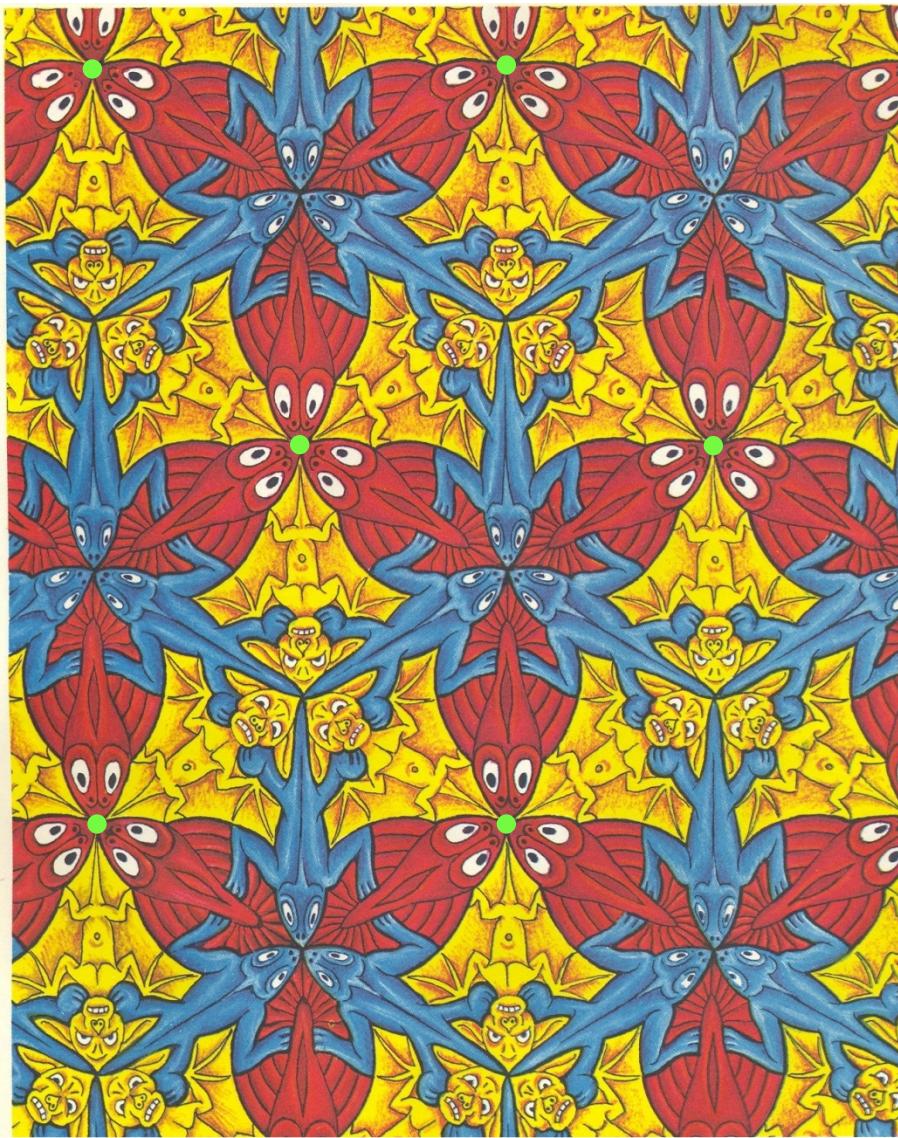
A 3D  
translationally  
periodic  
arrangement  
of points

# Relation between crystal and lattice?

Crystal = Lattice + Motif

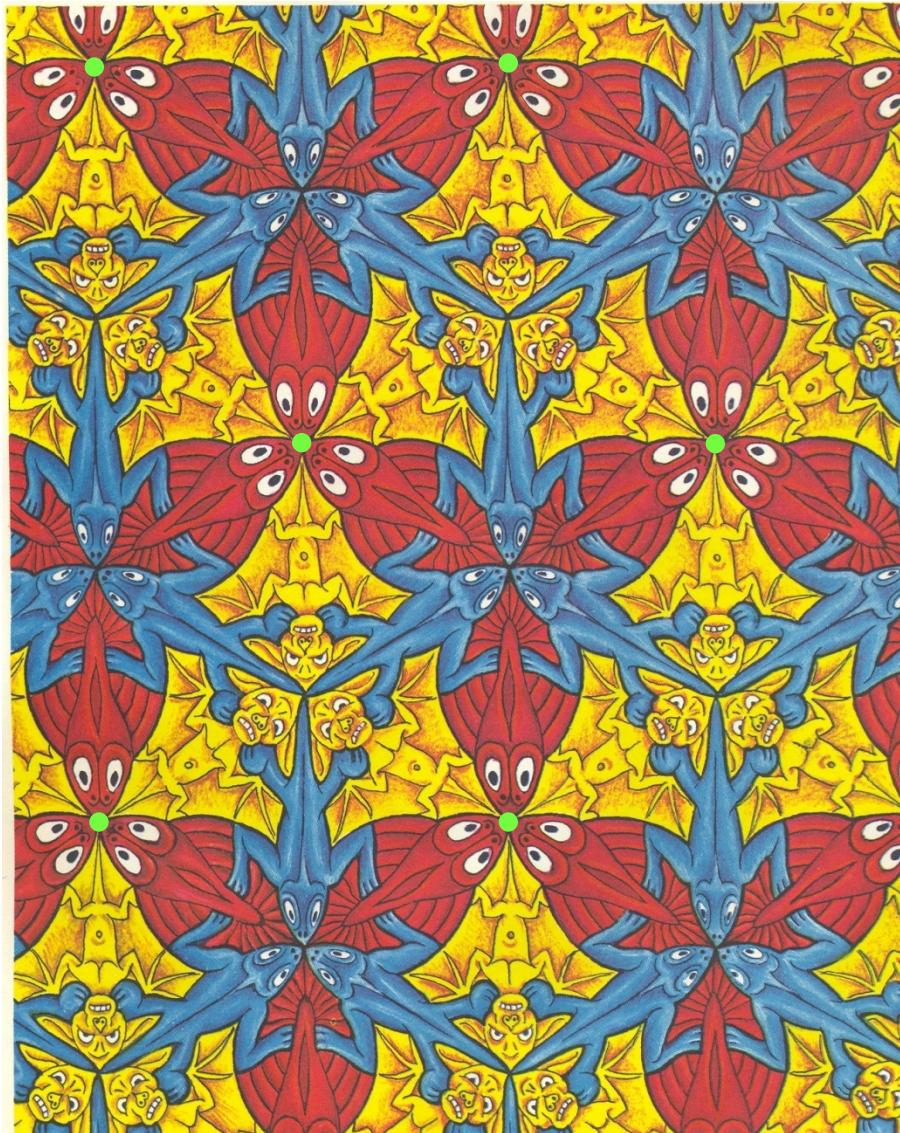
Motif or basis: an atom or a group of atoms associated with each lattice point

# Air, Water and Earth by M.C.Esher



# Air, Water and Earth by M.C.Esher

Every periodic pattern (and hence a crystal) has a unique lattice associated with it



**1965**

Symmetry Aspects of M. C. Escher's  
Periodic Drawings

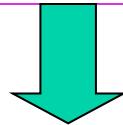
**Macgillavry, Caroline H. (Professor of  
Chemical Crystallography, Univ. of  
Amsterdam)**

**International Union of Crystallography**

# Escher: *Art* or Science?

Prof. Sanil's Class, Every semester since 2008  
Bangalore, May 26, 2009

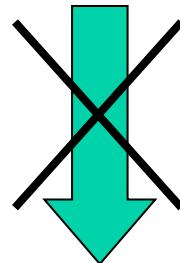
The six lattice parameters  
 $a, b, c, \alpha, \beta, \gamma$



The unit cell of the lattice



lattice



+ Motif

crystal



# Hexagonal Close Packed (HCP) Lattice?

Crystal System	Bravais Lattices			
1. Cubic	P	I	F	
2. Tetragonal	P	I		
3. Orthorhombic	P	I	F	C
4. Hexagonal	P			
5. Trigonal	P			
6. Monoclinic	P			C
7. Triclinic	P			

## ~~HCP Lattice~~

Only hexagonal lattice is Simple hexagonal

HCP crystal: ..ABAB.. Stacking of closed-packed layers

A and B not translationally equivalent

HCP crystal = Hexagonal *P* lattice

+ 2 atom motif (1A & 1B)



Web

Images

Maps

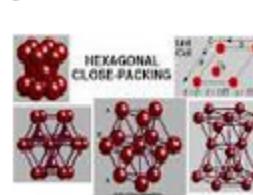
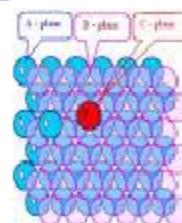
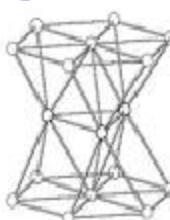
Books

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On 21.03.2013

[Images for "hexagonal close packed lattice" - Report images](#)[\[PDF\] 1. Hexagonal close-packed lattice a\) Verify that the ba...](#)<https://wiki.oulu.fi/download/attachments/15698835/ex2.pdf?...1...>File Format: PDF/Adobe Acrobat - [Quick View](#)

763628S CONDENSED MATTER PHYSICS Problem Set 2 Spring 2012. 1.

**Hexagonal close-packed lattice** a) Verify that the basis vectors  $a_1 = (a, 0, 0)$ ,  $a_2 = (a ...$ [Hexagonal-close-packed lattice: Ground state and phase tr...](#)[pre.aps.org](http://pre.aps.org) > Journals > Phys. Rev. E > Volume 85 > Issue 4by DT Hoang - 2012 - [Related articles](#)

Apr 9, 2012 – We study the ground state (GS) and the phase transition in a hexagonal close packed lattice with both W and Ising models by using



"diamond cubic lattice"

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### Crystal Structure

28 Jan 2010 ... Figure 8: Unit cell structure of a **diamond cubic lattice** showing the two interpenetrating face-centered cubic lattices. ...  
[cnx.org](#) > Content - Cached - Similar

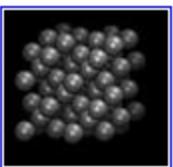
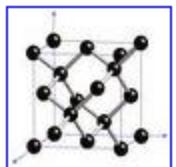
### Diamond Lattice Unit Cell Molecular Model Kit

This diamond lattice molecular model kit shows the CCP cubic crystal unit cell structure clearly and stands over 200mm tall.  
[www.indigo.com/models/gphmodel/diamond-model-W.html](#) - Cached - Similar

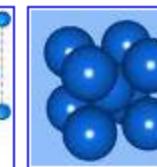
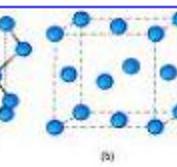
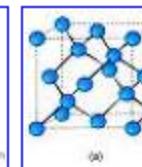
### Diamond cubic Sn-rich nanocrystals: synthesis, microstructure and ...

by R Ragan - 2005 - Related articles  
beled 6.3 Å and 4.8 Å in Fig. 2d is 68.5. • rather than 90. • as expected for the **diamond cubic lattice**. The deviation was at- ...  
[www.springerlink.com/index/JLNUQ3863823GP28.pdf](#) - Similar

### Images for "diamond cubic lattice" - Report images



$$\begin{aligned} \text{For } \alpha = 0, \beta = 0, \gamma = 0, \text{ then } \frac{\partial f}{\partial \alpha} = 0 \\ \Rightarrow \frac{\partial f}{\partial \alpha} = \frac{\partial}{\partial \alpha} \left[ \frac{1}{2} \exp[\alpha] \left( \frac{\partial^2 f}{\partial \alpha^2} + \frac{\partial^2 f}{\partial \beta^2} \right) \right] \\ = \frac{1}{2} \exp[\alpha] \left( \frac{\partial^2 f}{\partial \alpha^2} + \frac{\partial^2 f}{\partial \beta^2} \right) = 0 \\ \Rightarrow \frac{\partial^2 f}{\partial \alpha^2} + \frac{\partial^2 f}{\partial \beta^2} = 0 \end{aligned}$$



### XMD - Molecular Dynamics Program: Fill Command

9.2 FILL Example 2: Creating an **Diamond Cubic Lattice** ... The **diamond cubic lattice** is made by duplicating a pair of atoms using the repeating cell vectors ...  
[xmd.sourceforge.net/doc/manual/xmd-9.html](#) - Cached

There is no  
diamond  
cubic  
lattice.

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About 44,800 results (0.22 seconds)

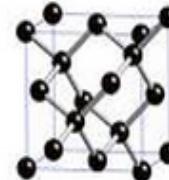
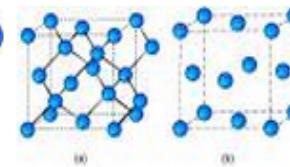
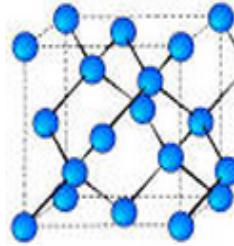
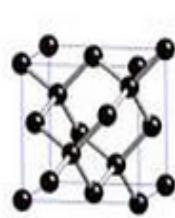
### [Diamond cubic - Wikipedia, the free encyclopedia](#)

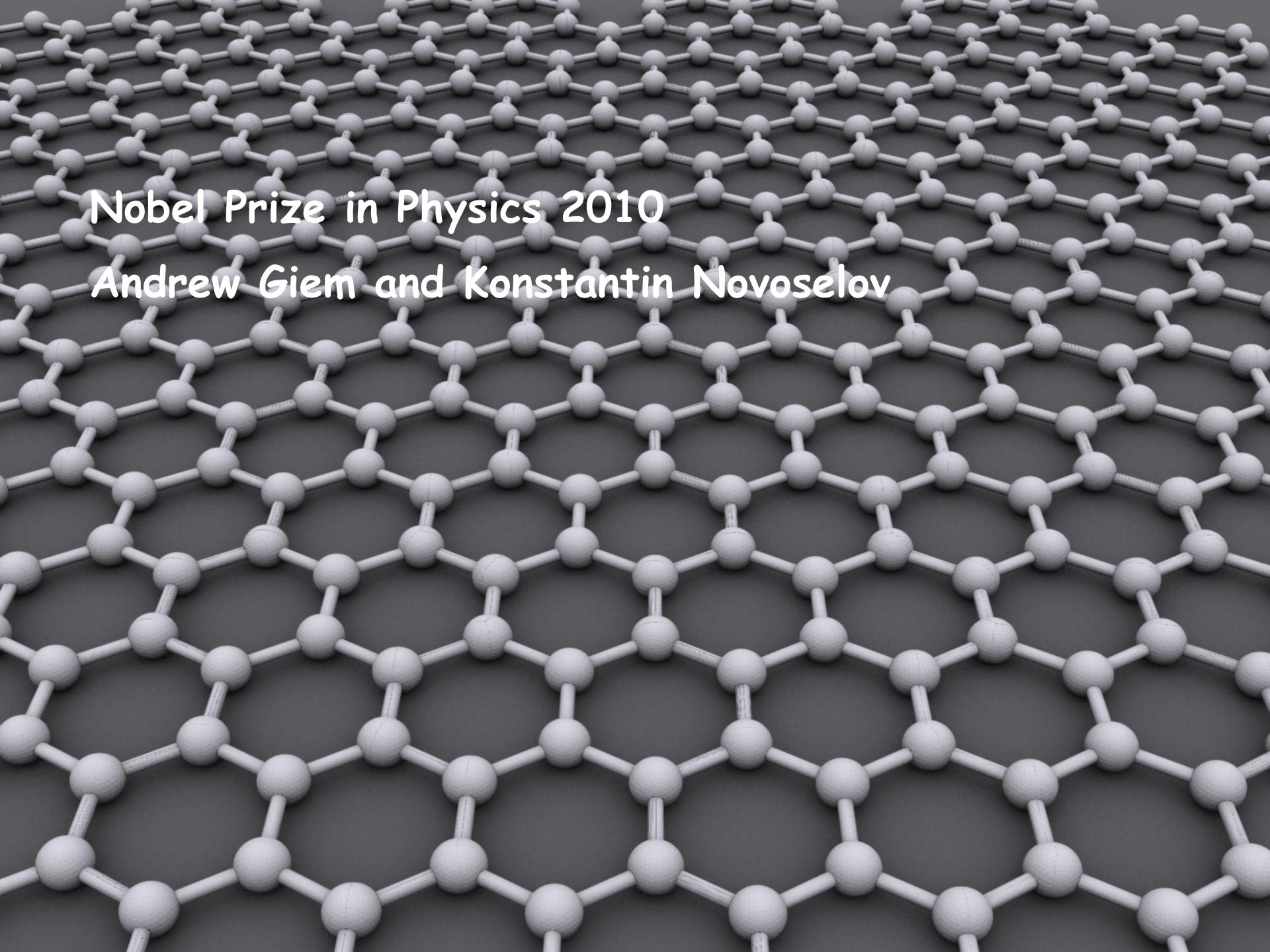
[en.wikipedia.org/wiki/Diamond\\_cubic](https://en.wikipedia.org/wiki/Diamond_cubic)

Media related to Diamond cubic at Wikimedia Commons; diamond 3D animation · Software to construct self avoiding random walks on the **diamond cubic lattice** ...

[Crystallographic structure](#) - [Mathematical structure](#) - [Manufacturing considerations](#)

### [Images for "diamond cubic lattice"](#) - Report images



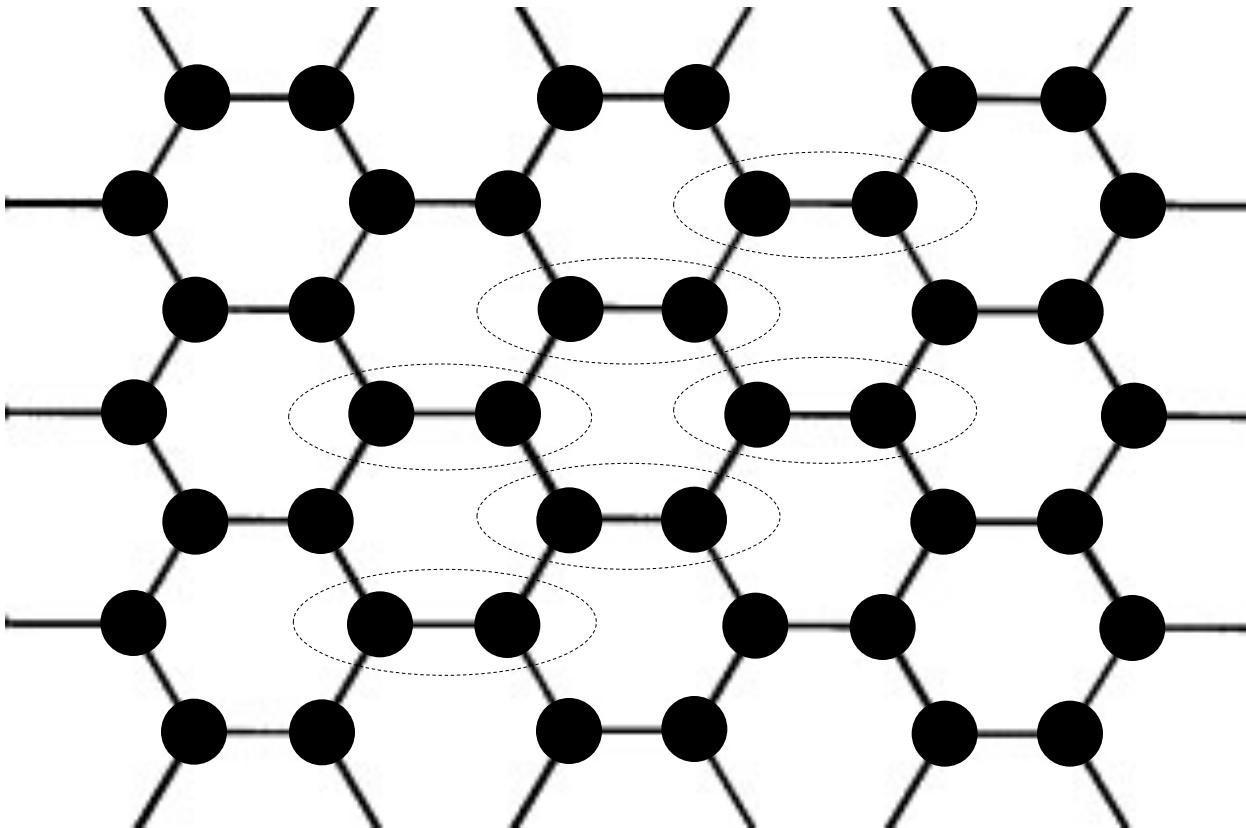


Nobel Prize in Physics 2010

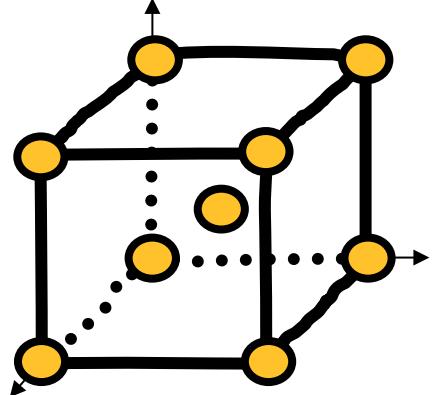
Andrew Giem and Konstantin Novoselov

# Crystal structure of Graphene

Graphene crystal = hexagonal Lattice + 2 atom motif



## Monatomic Body-Centred Cubic (BCC) crystal

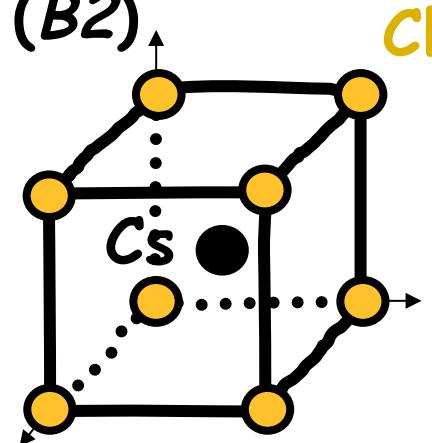


Corner and body-centres have the same neighbourhood

Lattice: bcc

Motif: 1 atom 000

## CsCl crystal (B2)



Corner and body-centred atoms *do not* have the same neighbourhood

Lattice: simple cubic

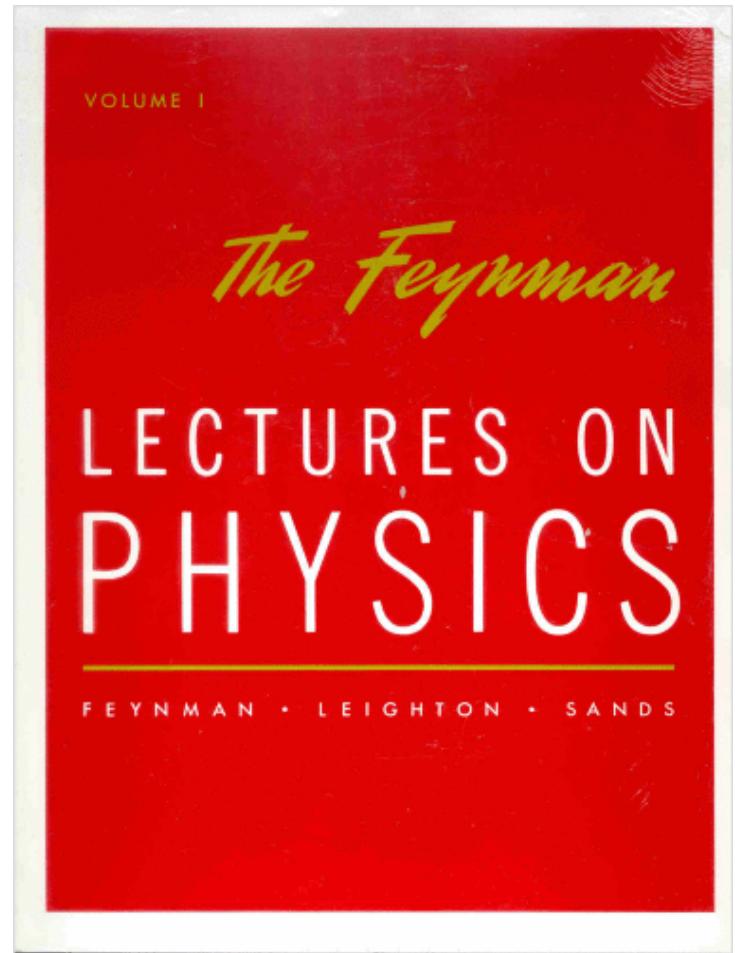
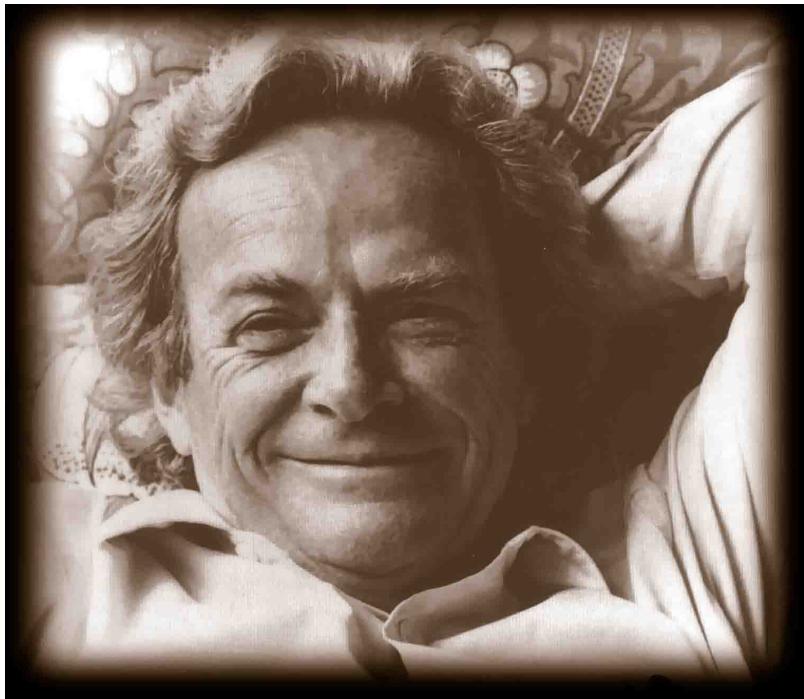
~~BCC~~

Feynman!

Motif: two atoms

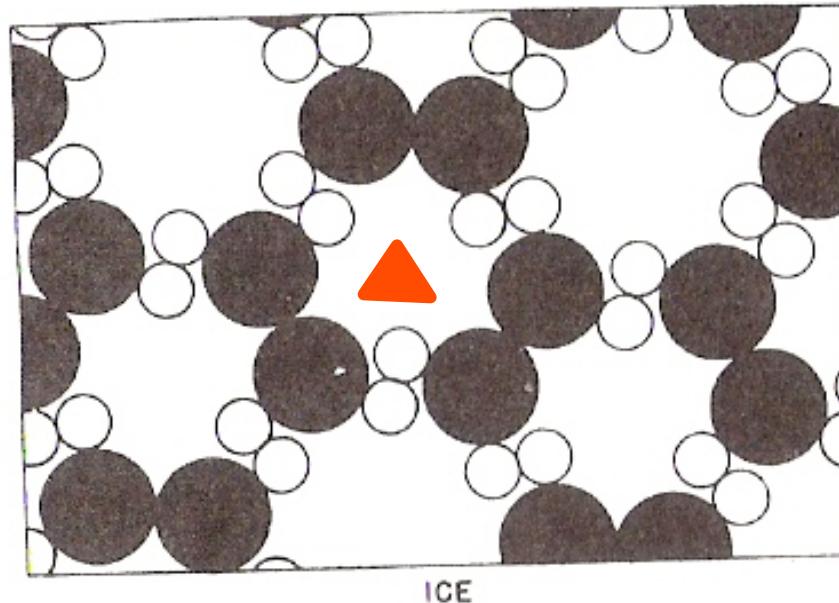
Cl 000; Cs  $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

# Richard P. Feynman



Nobel Prize in Physics, 1965

# Feynman's Lectures on Physics Vol 1 Chap 1 Fig. 1-4

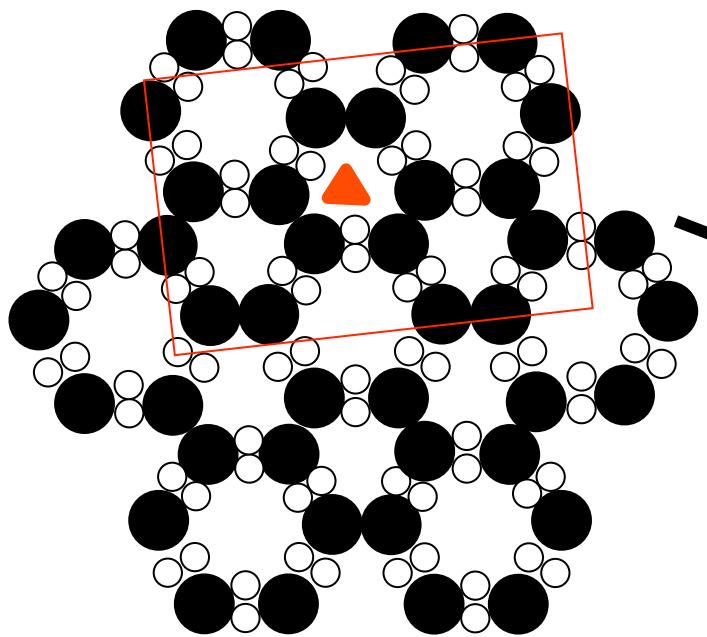


Hexagonal symmetry

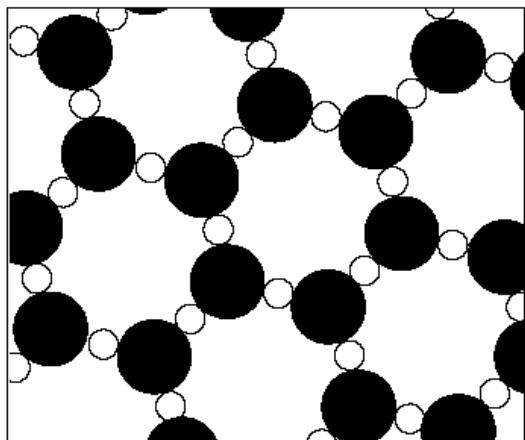
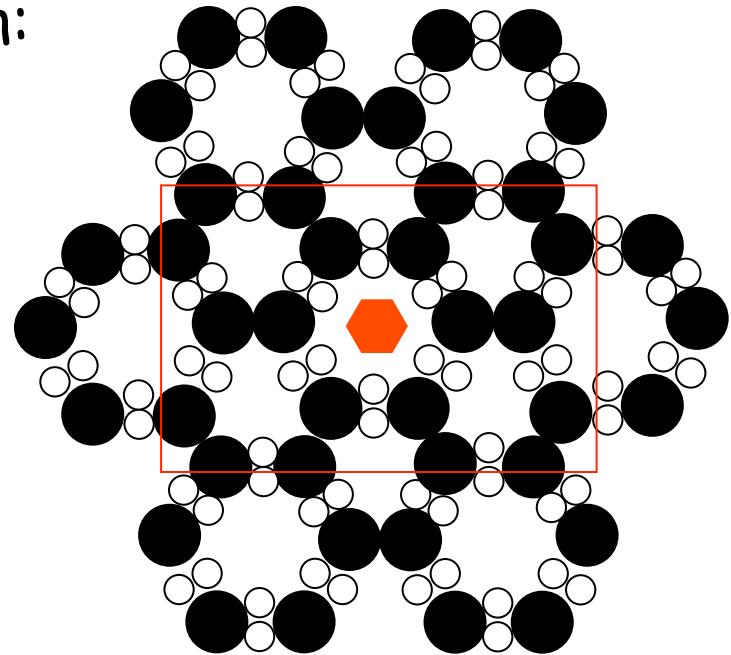
$$\theta = \frac{360}{6} = 60^\circ$$

Figure 1-4

“Fig. 1-4 is an invented arrangement for ice, and although it contains many of the correct features of the ice, it is not the true arrangement. One of the correct features is that there is a part of the symmetry that is hexagonal. You can see that if we turn the picture around an axis by ~~120°~~, the picture returns to itself.”



Correction:  
Shift the  
box



ICE

One suggested  
correction:

But gives H:O = 1.5 : 1

Figure 1-4

## Summary

**Lattice:** translationally periodic set of points.

**Crystal:** translationally periodic set of atoms.

**Motif or basis:** an atom or group of atoms associated with each lattice point

$$\text{Crystal} = \text{Lattice} + \text{Motif}$$

HCP is a crystal structure and not a lattice.

7 crystal system and 14 Bravais: symmetry (not unit cell)

**7 crystal system:**  
lattices

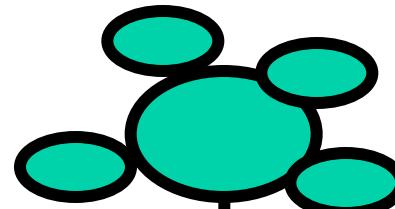
7 different point groups of

**14 Bravais lattices:** 14 different space groups of lattices

We hope this book will help in clearing up the confusion that many solid state scientists encounter when starting to study solid state symmetry. How many well-established scientists still believe that all cubic crystals must have axes of fourfold symmetry, for example? In a similar vein how many of them would define a crystal system according to the lengths of the unit cell axes and their interaxial angles? How many know which character tables to use for a crystal that has a glide plane or a screw axis? If we can clarify a few of these kinds of problems, and nothing else, we shall feel that the writing of this have been worthwhile.

Burns and Glazer in the preface of their book  
“*Space Groups for Solid state Scientists*”

QUESTIONS?



# Miller Indices

# Miller Indices of Directions

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

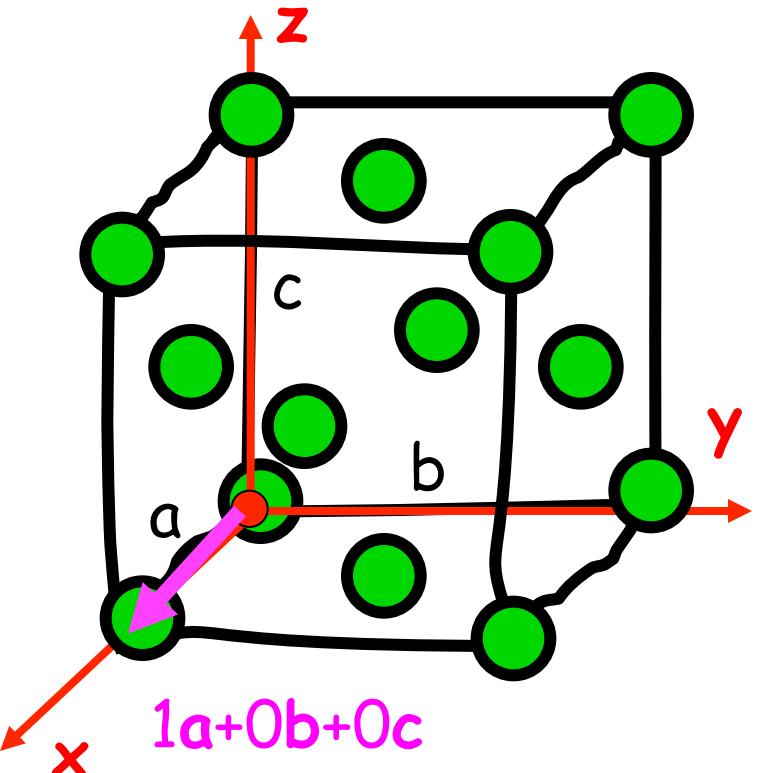
2. Choose a coordinate system with axes parallel to the unit cell edges.

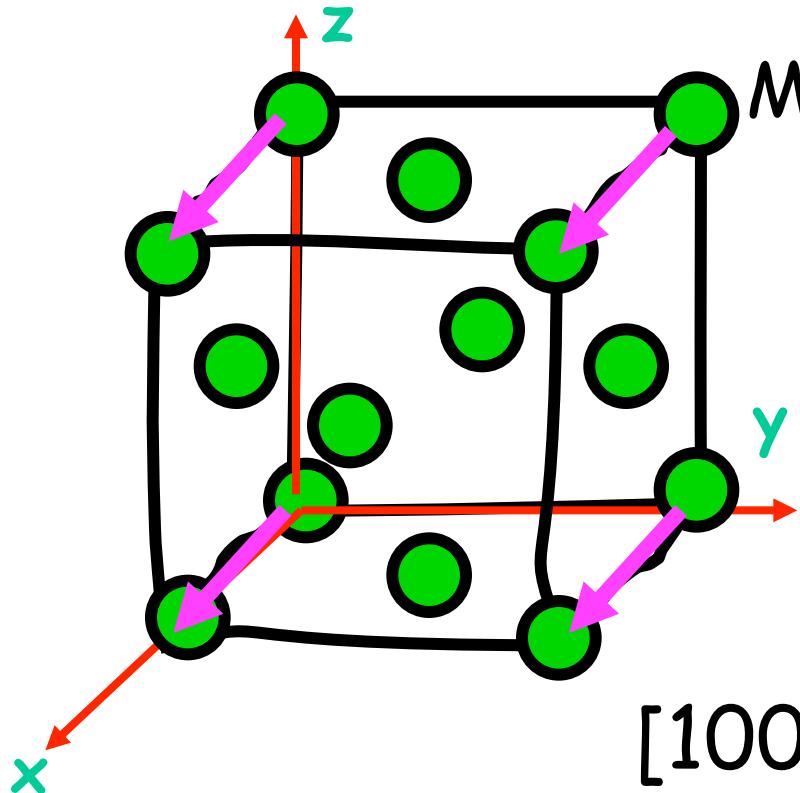
3. Find the coordinates of another point on the direction in terms of  $a$ ,  $b$  and  $c$

$1, 0, 0$

4. Reduce the coordinates to smallest integers.  $1, 0, 0$

5. Put in square brackets  $[100]$

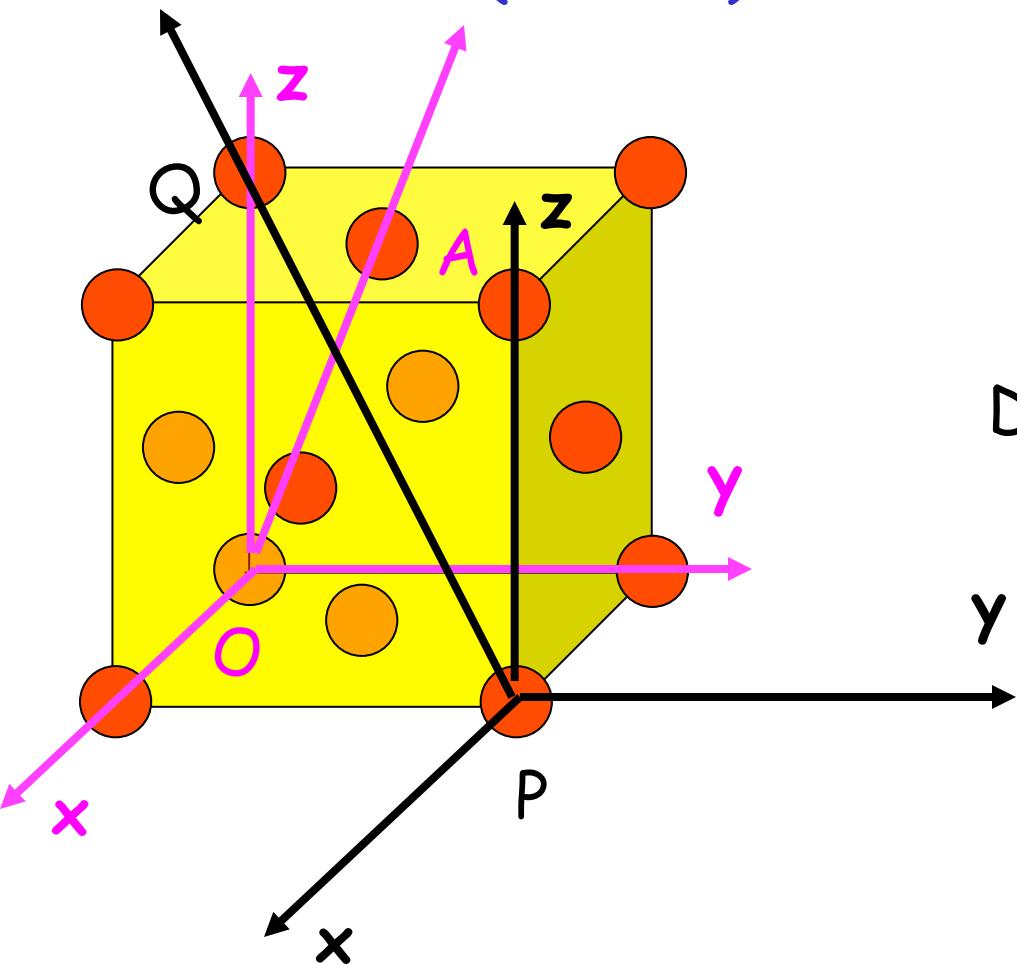




Miller indices of a direction:  
only the orientation  
not its position or sense

All parallel directions have the  
same Miller indices

## Miller Indices of Directions (contd.)



Direction OA

$$OA = \frac{1}{2} \mathbf{a} + \frac{1}{2} \mathbf{b} + 1 \mathbf{c}$$

$$\frac{1}{2}, \frac{1}{2}, 1$$

$$[1 \ 1 \ 2]$$

Direction PQ

$$PQ = -1 \mathbf{a} - 1 \mathbf{b} + 1 \mathbf{c}$$

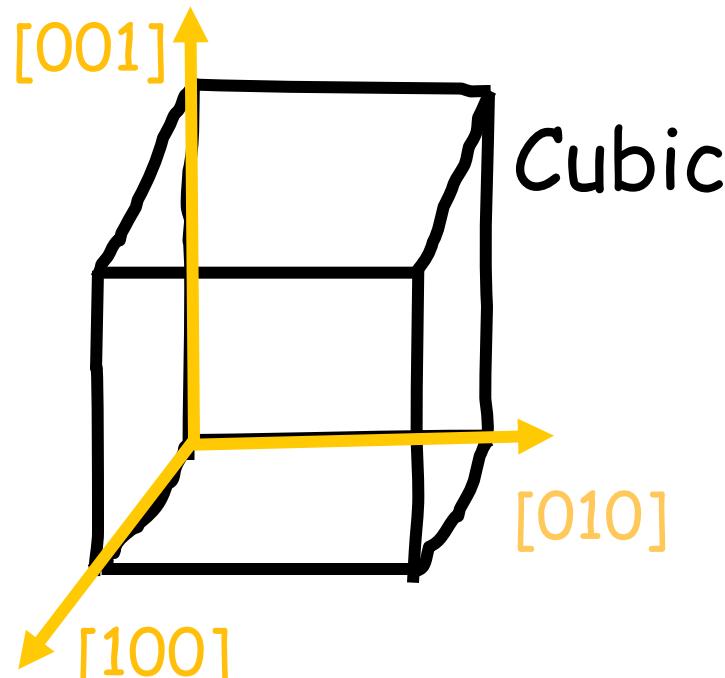
$$-1, -1, 1$$

$$[\overline{1}\overline{1}1]$$

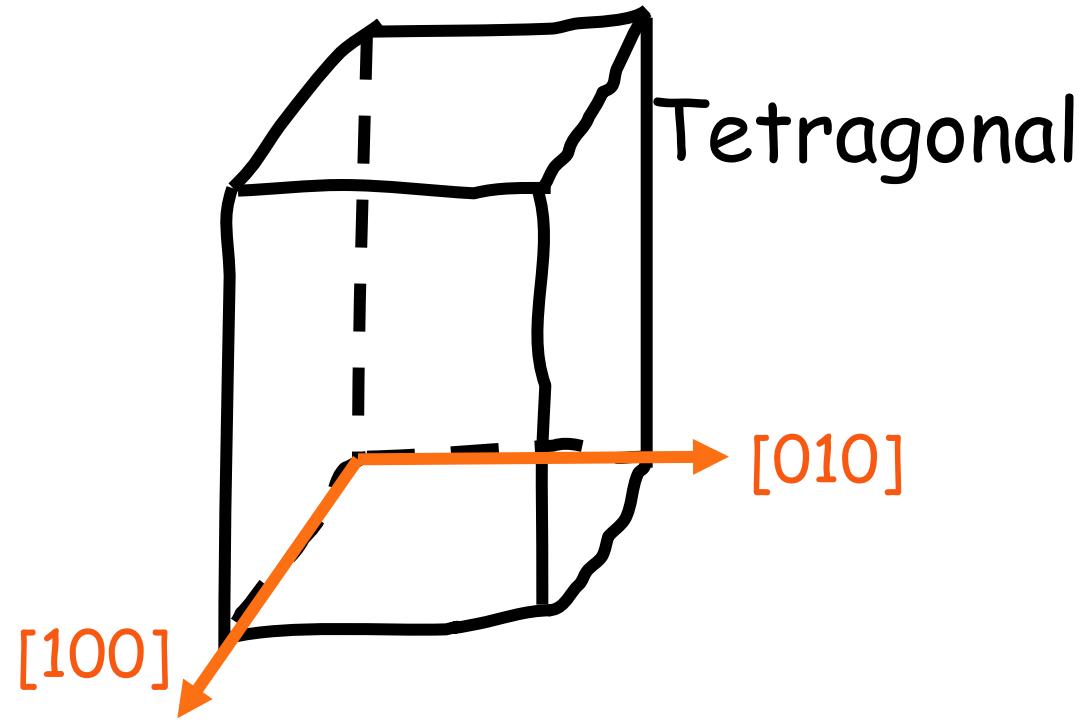
-ve steps are shown as bar over the number

# 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



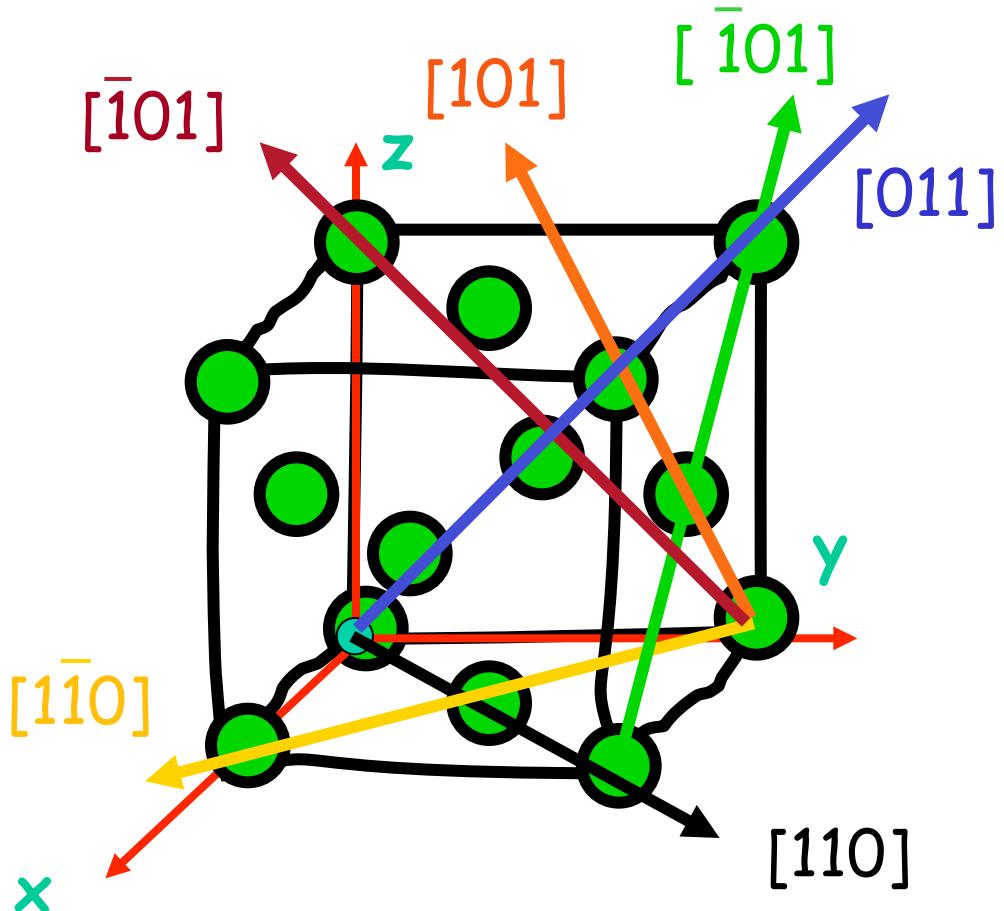
$$\langle 100 \rangle_{cubic} = [100], [010], [001]$$



$$\langle 100 \rangle_{tetragonal} = [100], [010]$$

# Miller indices of slip directions in CCP

Slip directions = close-packed directions = face diagonals



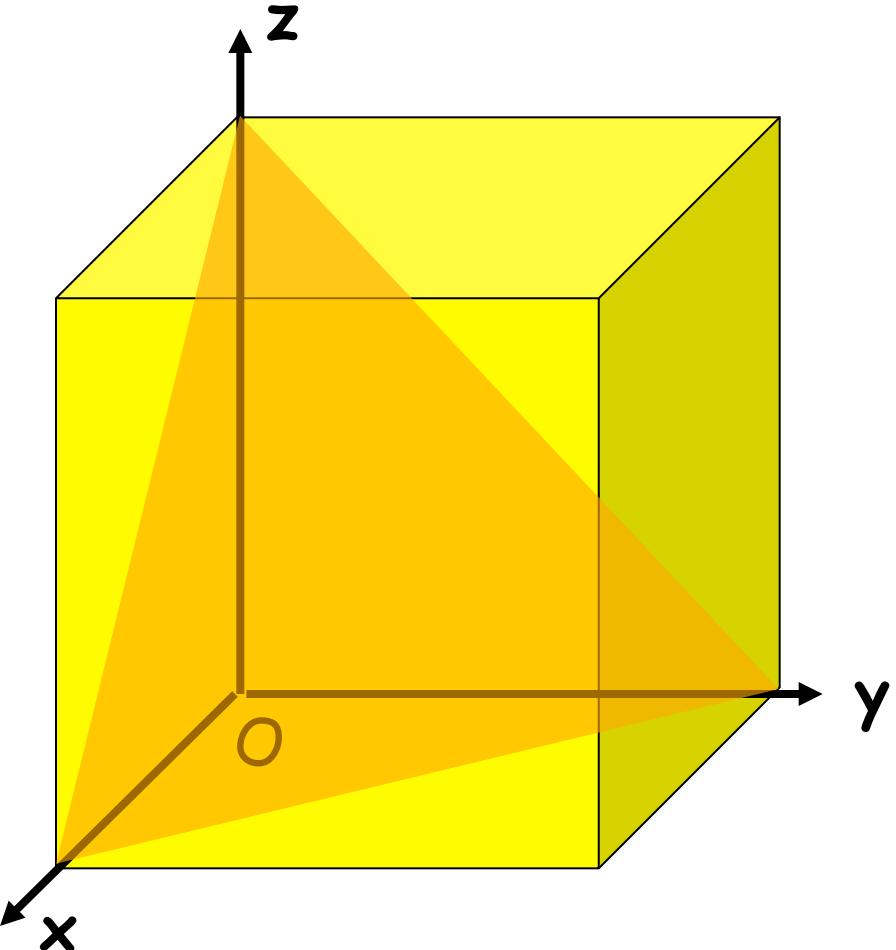
Six slip directions:

[110]	$\bar{[1}10]$
[101]	$\bar{[1}01]$
[011]	$\bar{[1}01]$

All six slip  
directions in ccp:

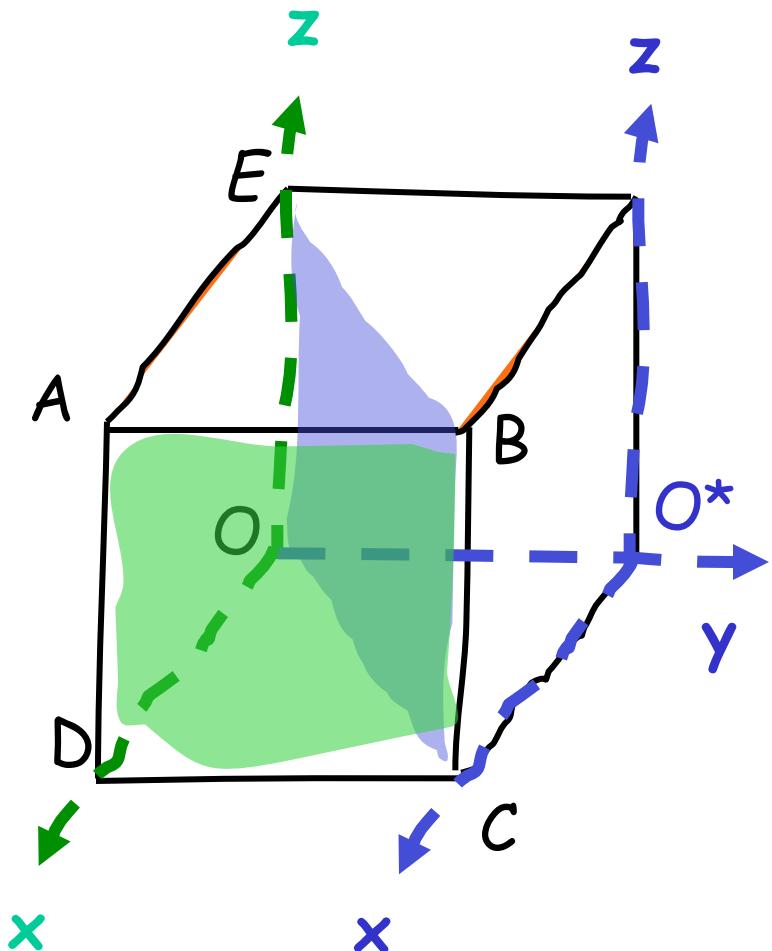
$\langle 110 \rangle$

## Miller Indices for planes



1. Select a crystallographic coordinate system with origin not on the plane
2. Find intercepts along axes  
 $1 \ 1 \ 1$
3. Take reciprocal       $1 \ 1 \ 1$
4. Convert to smallest integers in the same ratio  
 $1 \ 1 \ 1$
5. Enclose in parenthesis  
 $(111)$

## Miller Indices for planes (contd.)



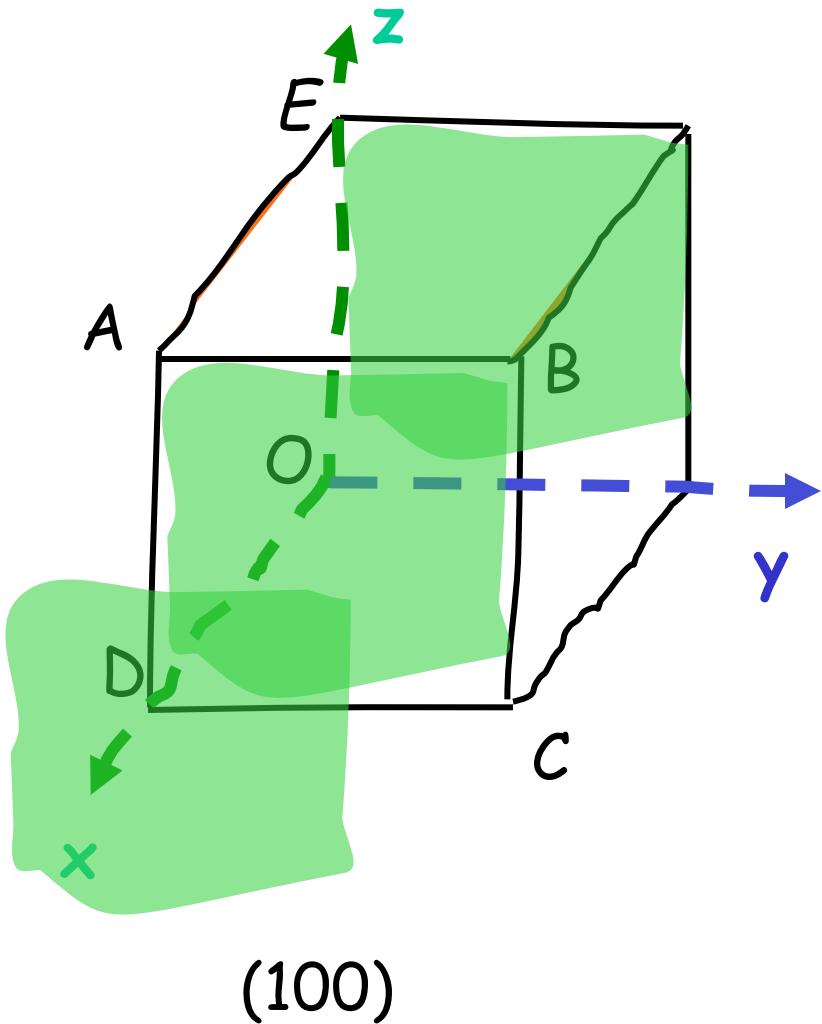
Plane	$ABCD$	$OCBE$
origin	O	$O^*$
intercepts	1 $\infty$ $\infty$	1 -1
reciprocals	1 0 0	$\infty$
Miller Indices	(1 0 0)	1 -1 0

Zero represents that the plane is parallel to the corresponding axis

Bar represents a negative intercept

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

All parallel planes have the same Miller Indices

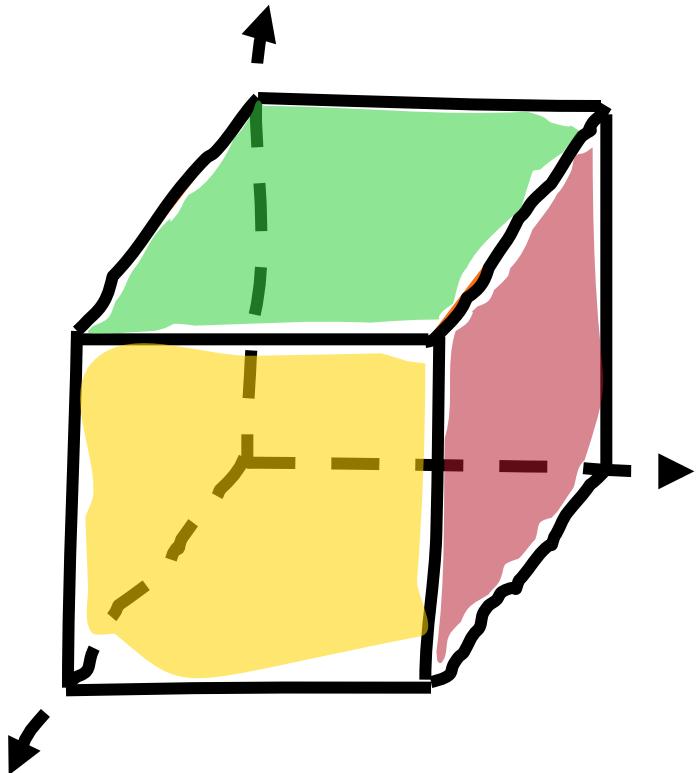


$$(h k l) \equiv (\bar{h} \bar{k} \bar{l})$$

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

## 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)

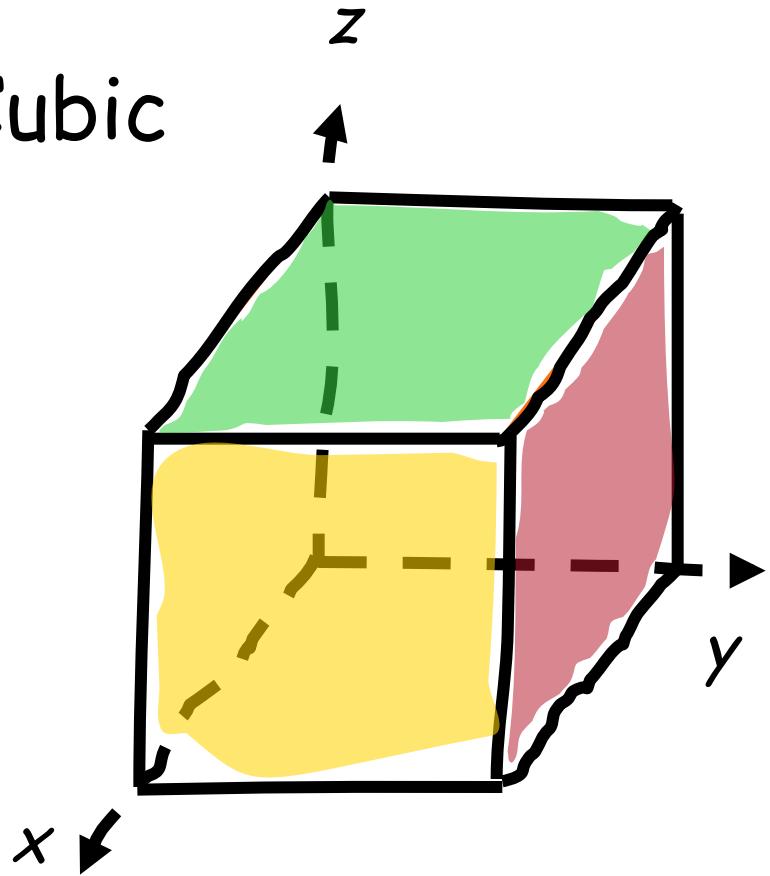
Left and right faces: (010)

Top and bottom faces: (001)

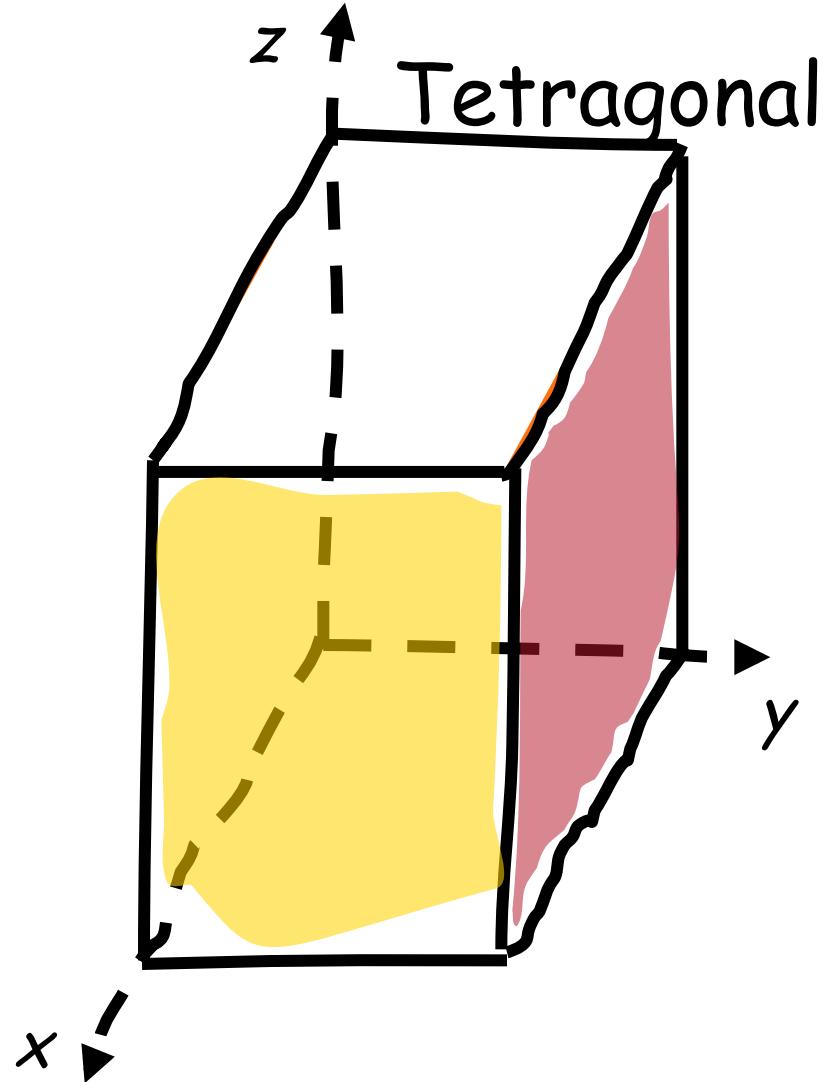
$$\{100\} = (100), (010), (001)$$

## Miller indices of a family of symmetry related planes

Cubic



$$\{100\}_{\text{cubic}} = (100), (010), (001)$$

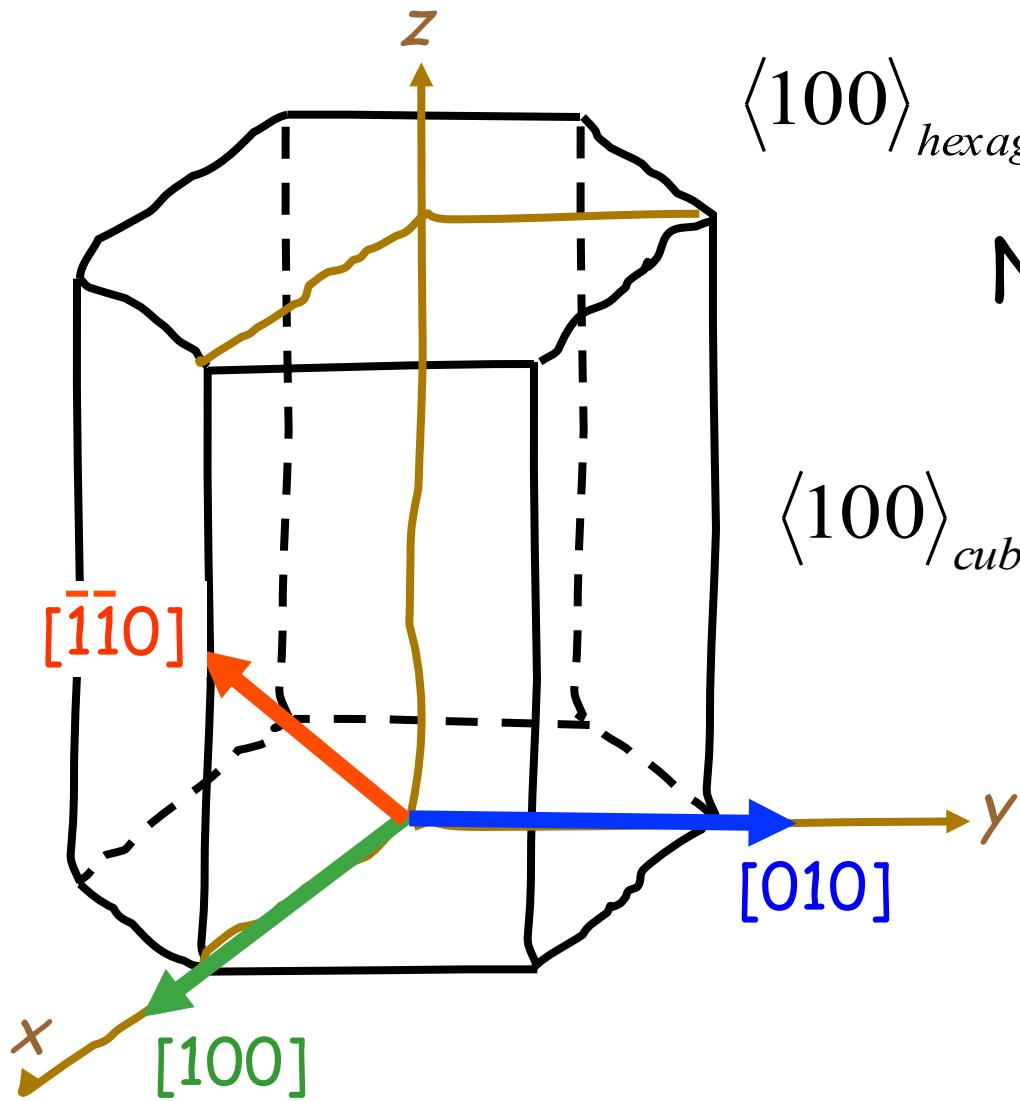


$$\{100\}_{\text{tetragonal}} = (100), (010)$$

~~(001)~~

64/17  
61

# Symmetry related directions in the hexagonal crystal system



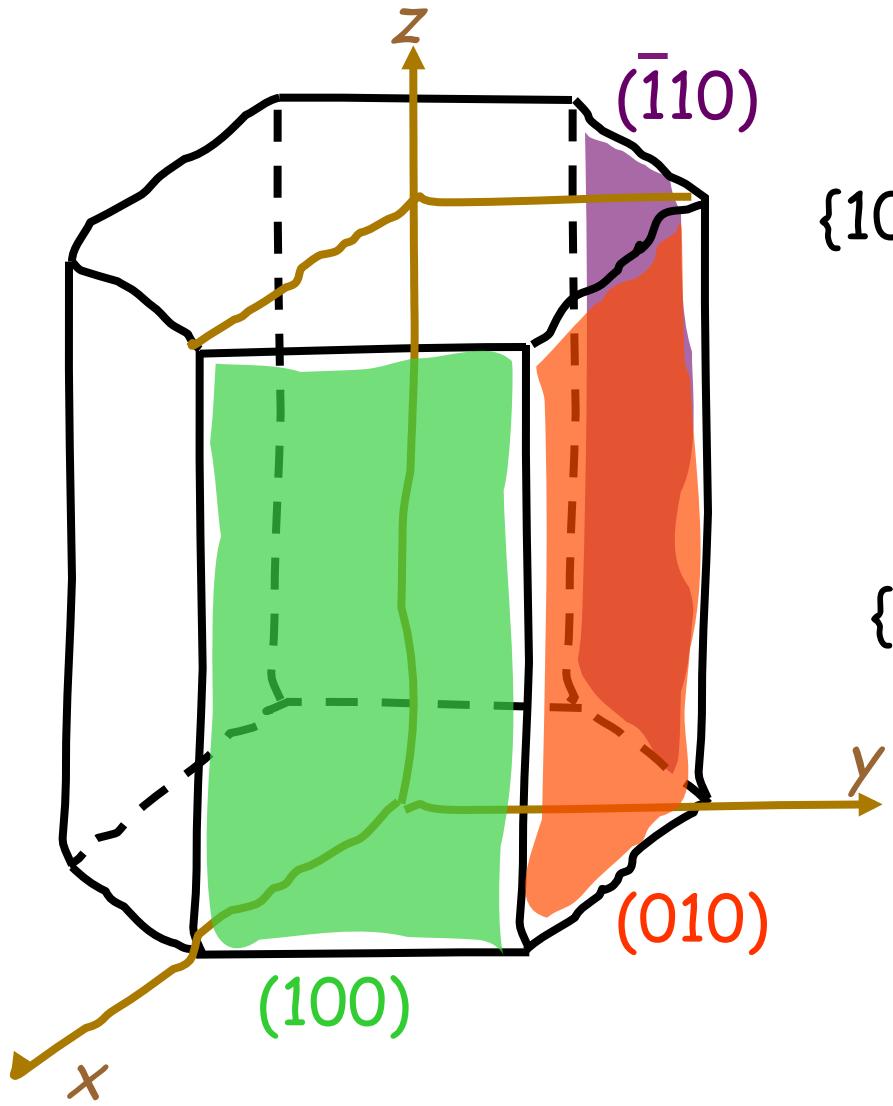
$$\langle 100 \rangle_{hexagonal} = [100], [010], [\bar{1}\bar{1}0]$$

Not permutations

$$\langle 100 \rangle_{cubic} = [100], [010], [001]$$

Permutations

# Symmetry related planes in the hexagonal crystal system



$$\{100\}_{\text{hexagonal}} = (100), (010), (\bar{1}10)$$

Not permutations

$$\{100\}_{\text{cubic}} = (100), (010), (001)$$

Permutations

Problem:

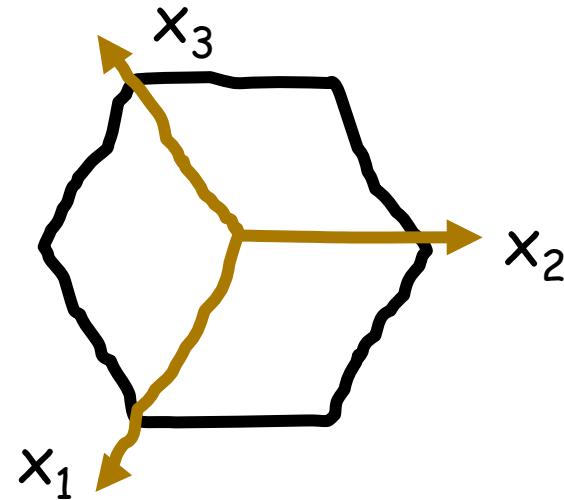
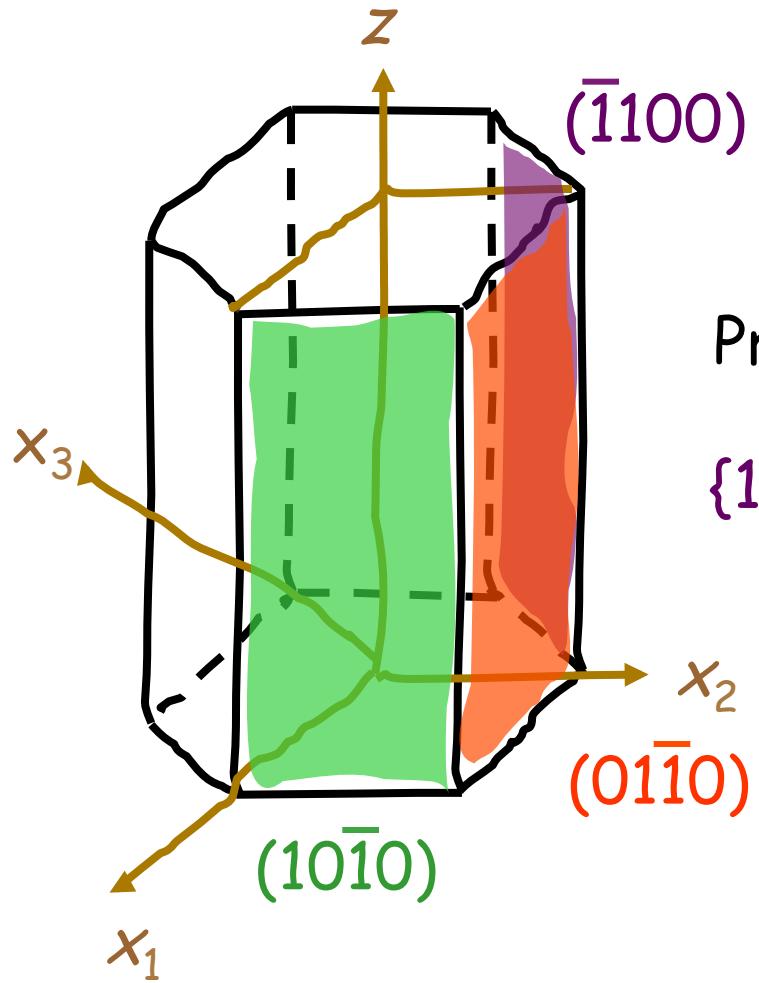
In hexagonal system symmetry related planes and directions do **NOT** have Miller indices which are *permutations*

Solution:

Use the four-index Miller-Bravais Indices instead

# Miller-Bravais Indices of Planes

Introduce a fourth axis in  
the basal plane



Prismatic planes:

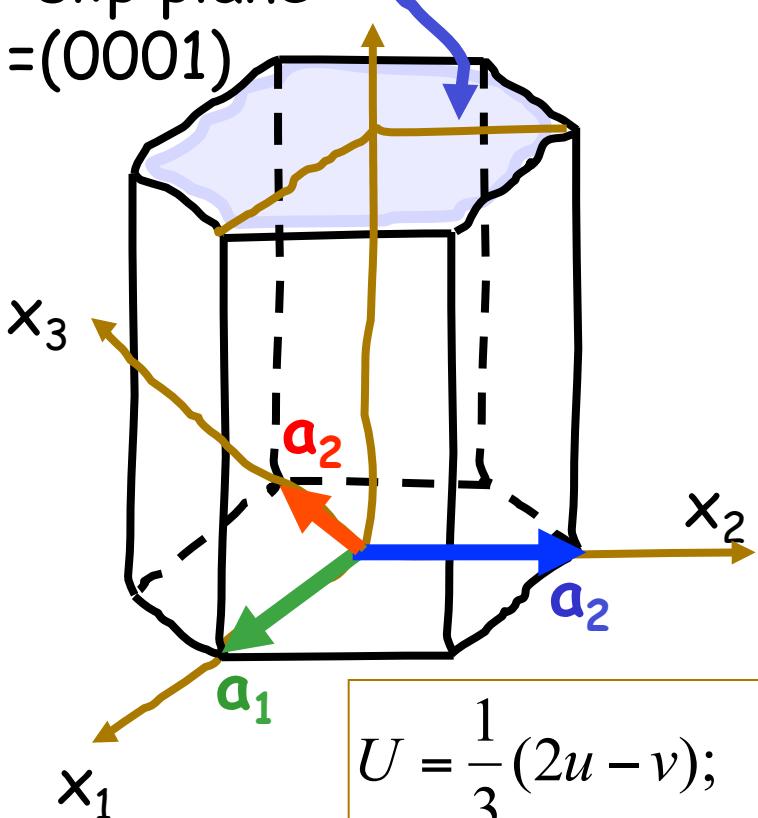
$$\{1\bar{1}00\} = (10\bar{1}0) \quad (01\bar{1}0) \quad (\bar{1}100)$$

$(hkl) \Rightarrow (hkil)$  with  $i = -(h+k)$

# Miller-Bravais Indices of Directions in hexagonal crystals $[uvw] \Rightarrow [UVTW]$

Vectorially  $\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3 = 0$

Basal plane  
= slip plane  
=(0001)



Require that:  $U + V + T = 0$

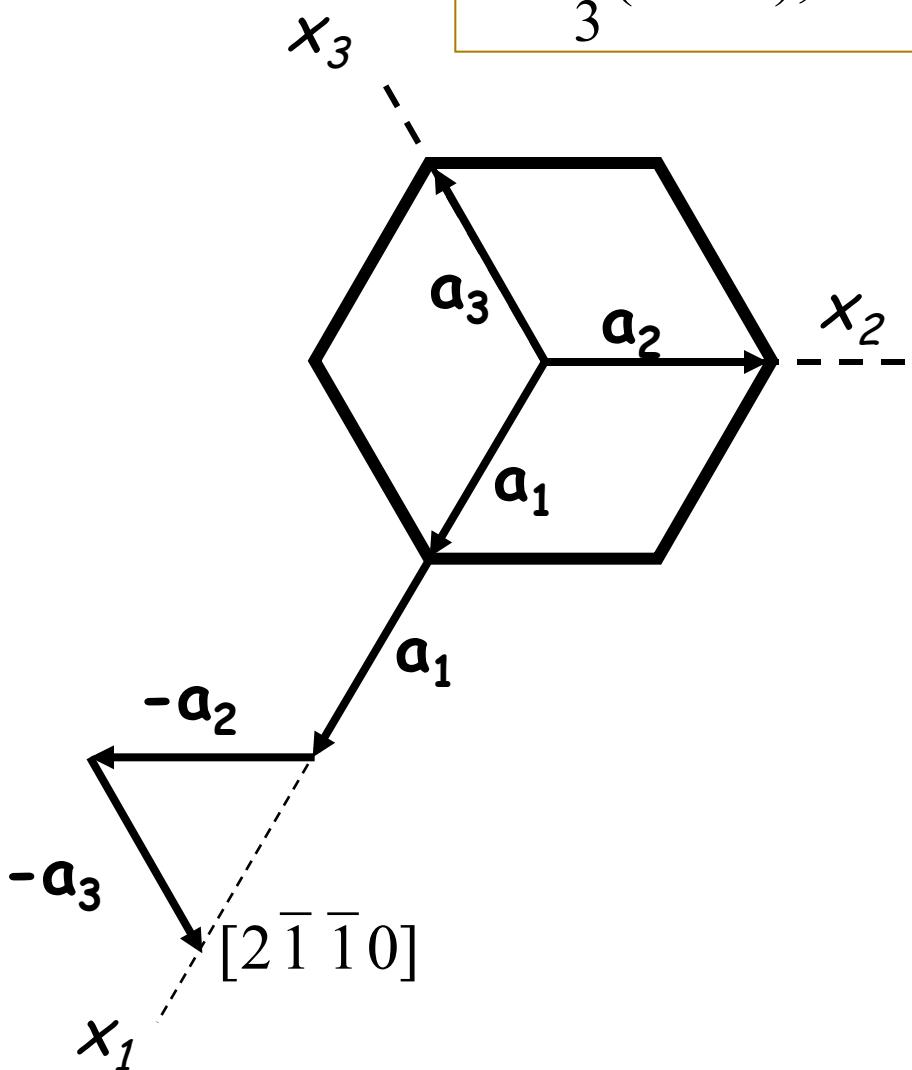
$$U\mathbf{a}_1 + V\mathbf{a}_2 + T\mathbf{a}_3 + W\mathbf{c} = u\mathbf{a}_1 + v\mathbf{a}_2 + w\mathbf{c}$$



$$U = \frac{1}{3}(2u - v); \quad V = \frac{1}{3}(2v - u); \quad T = -(u + v); \quad W = w$$

# Miller-Bravais indices of slip directions in hcp crystal:

$$U = \frac{1}{3}(2u - v); \quad V = \frac{1}{3}(2v - u); \quad T = -(u + v); \quad W = w$$



$$x_1: [100] \Rightarrow \left[ \frac{2}{3} - \frac{1}{3} - \frac{1}{3} 0 \right] \equiv [2\bar{1}\bar{1}0]$$

$$x_2: [010] \Rightarrow \left[ -\frac{1}{3} \frac{2}{3} - \frac{1}{3} 0 \right] \equiv [\bar{1}2\bar{1}0]$$

$$x_3: [\bar{1}\bar{1}0] \Rightarrow \left[ -\frac{1}{3} - \frac{1}{3} \frac{2}{3} 0 \right] \equiv [\bar{1}\bar{1}20]$$

Slip directions in hcp

$\langle 2\bar{1}\bar{1}0 \rangle$

## Some IMPORTANT Results

# Weiss zone law

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

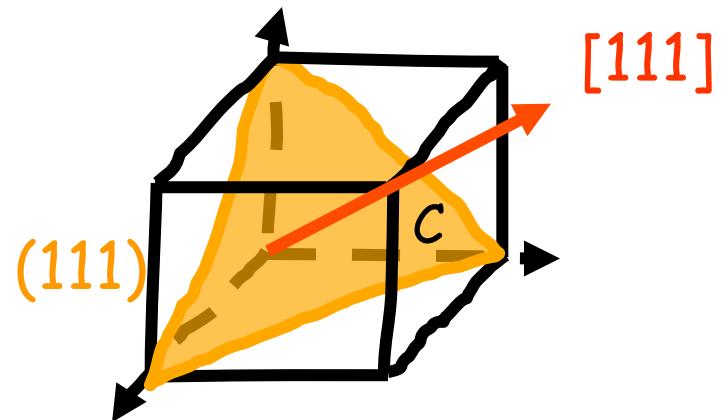
$$h u + k v + l w = 0$$

$$h U + k V + i T + l W = 0$$

*True for ALL crystal systems*

# CUBIC CRYSTALS

$$[hkl] \perp (hkl)$$

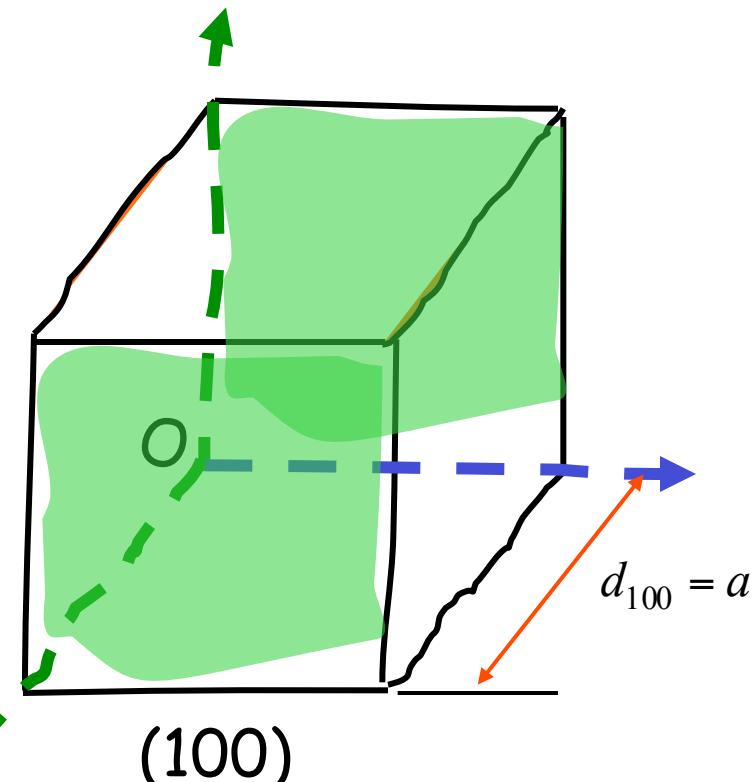


Angle between two directions  $[h_1k_1l_1]$  and  $[h_2k_2l_2]$ :

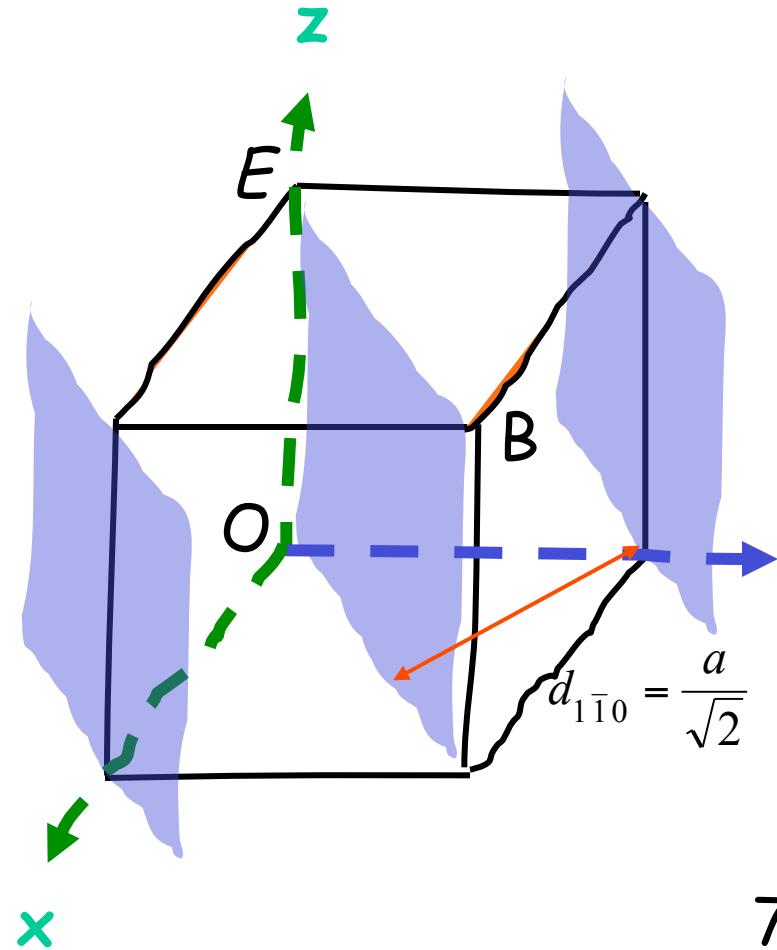
$$\cos \theta = \frac{h_1h_2 + k_1k_2 + l_1l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2} \sqrt{h_2^2 + k_2^2 + l_2^2}}$$

$d_{hkl}$

Interplanar spacing  
between 'successive' ( $hkl$ )  
planes passing through the  
**corners** of the unit cell



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



# X-Ray Diffraction Convention

**Normal convention:**

Miller indices (hkl) cannot have any common factor.

**X-Ray diffraction Convention:**

(hkl) is indices of a Bragg reflection (diffraction) peak.

It may have a common factor.

(nh,nk,nl) represents nth order reflection from (hkl)

(222) is the second order reflection from the (111)

# Vectors vs Directions:

Miller Indices of a direction

[110] is a direction along the face diagonal of a unit cell. It is not a vector of fixed length

Exception:

The Burger's vector

BCC       $\mathbf{b} = \frac{1}{2}\langle 111 \rangle$       A vector equal to half body diagonal

FCC       $\mathbf{b} = \frac{1}{2}\langle 110 \rangle$       A vector equal to half face diagonal

## Summary of Notation convention for Indices

[uvw]	Miller indices of a direction (i.e. a set of parallel directions)
$\langle uvw \rangle$	Miller indices of a family of symmetry related directions
(hkl)	Miller Indices of a plane (i.e. a set of parallel planes)
{hkl}	Miller indices of a family of symmetry related planes
[uvtw]	Miller-Bravais indices of a direction,
(hkil)	plane in a hexagonal system

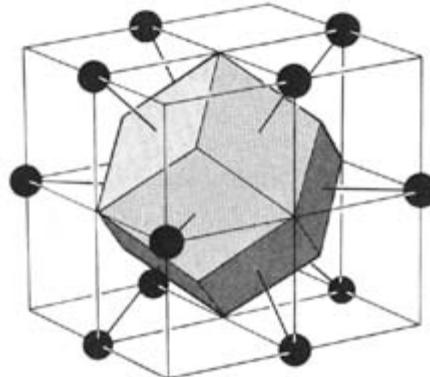
Thank you

# Appendices

- Wigner seitz unit cell (Voronoi cell)
- Brilluion zone
- Proof of crystallographic restriction
- Symmetry error in Feynman's lecture
- Quasicrystals
- Anisotropy of crystals: Neumann Principle
- Elastic anisotropy of crystals

# Wigner-Seitz Unit Cells (Voronoi Cells)

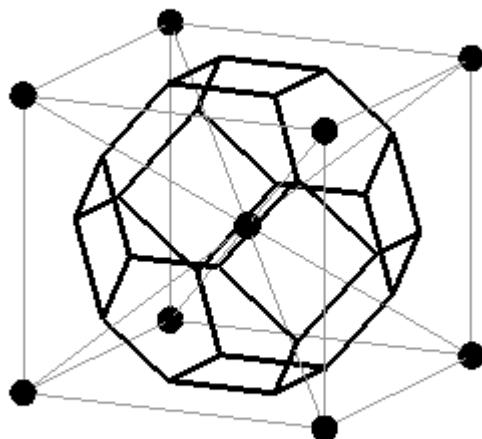
FCC



Rhombic Dodecahedron



BCC



Tetrakaidecahedron



Brillouin Zones are nothing but Wigner-Seitz cell of the reciprocal lattice

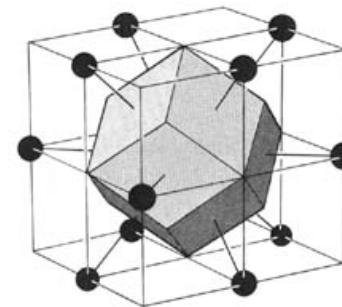
Real lattice

FCC

Reciprocal Lattice

BCC

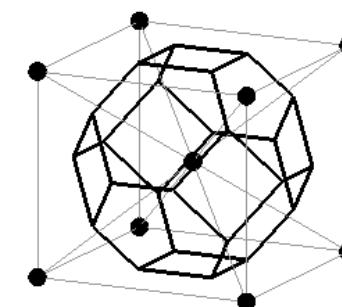
First Brillouin Zone



Rhombic Dodecahedron

BCC

FCC



Tetrakaidecahedron

# Proof of The Crystallographic Restriction

A rotation can be represented by a matrix  $T = \begin{pmatrix} t_{11} & t_{12} & t_{13} \\ t_{21} & t_{22} & t_{23} \\ t_{31} & t_{32} & t_{33} \end{pmatrix}$

$$\text{Trace}[T] = t_{11} + t_{22} + t_{33} = 2\cos\theta + 1$$

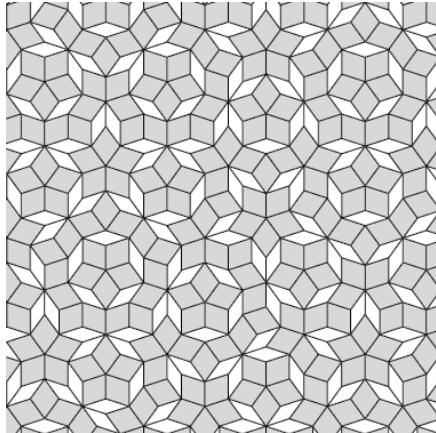
If  $T$  is a rotational symmetry of a lattice then all its elements must be integers (wrt primitive basis vectors)

$$\therefore 2\cos\theta + 1 = N \quad \Rightarrow -1 \leq N \leq 3$$

$N$	-1	0	1	2	3
$\theta$	$180^\circ$	$120^\circ$	$90^\circ$	$60^\circ$	$0^\circ$
$n$ -fold	2	3	4	6	1

# QUASICRYSTALS (1984)

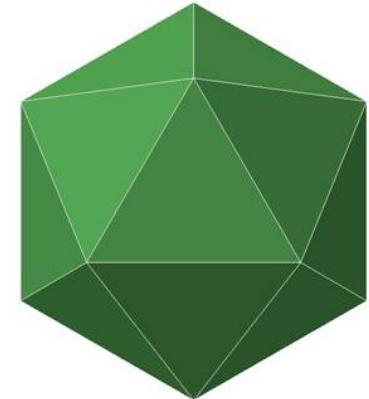
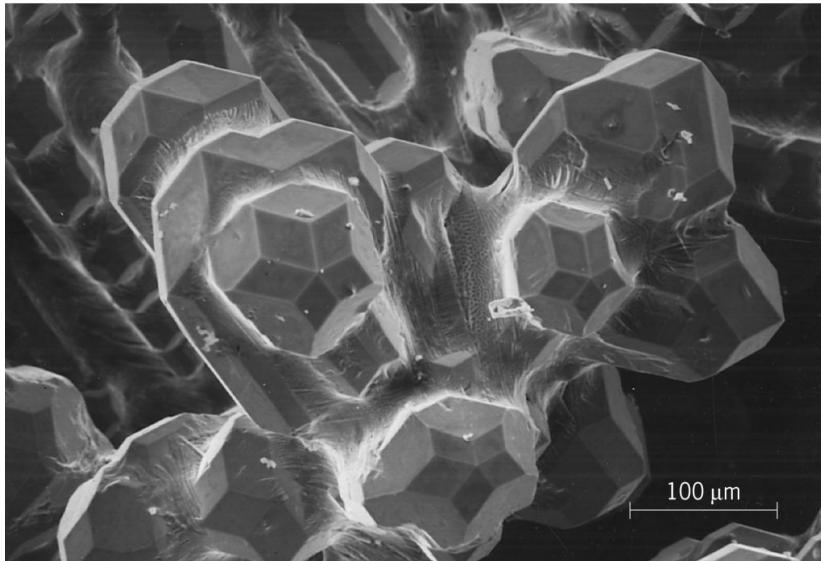
Icosahedral symmetry (5-fold symmetry)



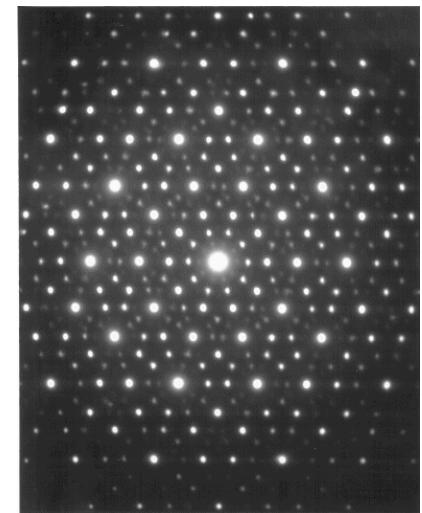
Penrose  
Tiling

External  
Morphology

Lack strict  
translational  
periodicity ->  
Quasiperiodic



Icosahedron



Diffraction  
Pattern

# Neumann's Principle

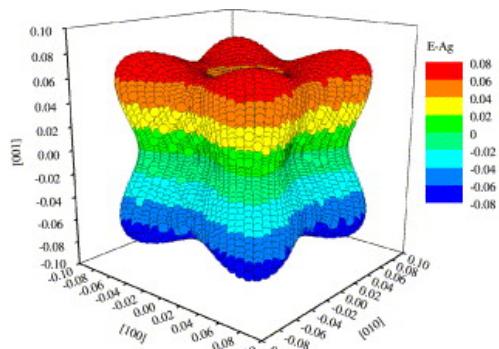
Symmetry elements of a physical property of a crystal must *include* all the symmetry elements of its point group (i.e., all its rotational axes and mirror planes).

Electrical resistance of a cubic crystal is isotropic (spherical symmetry)

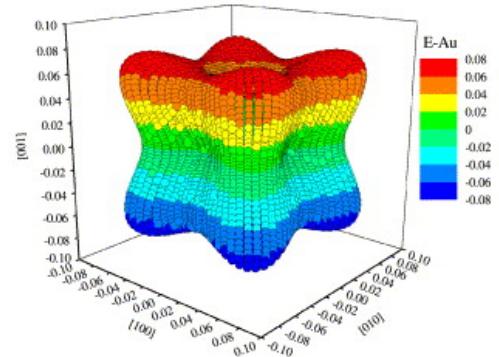
All properties that can be represented by tensors of rank up to 2 are isotropic for cubic crystals

# Elastic modulus (4<sup>th</sup>. Rank Tensor) is not isotropic

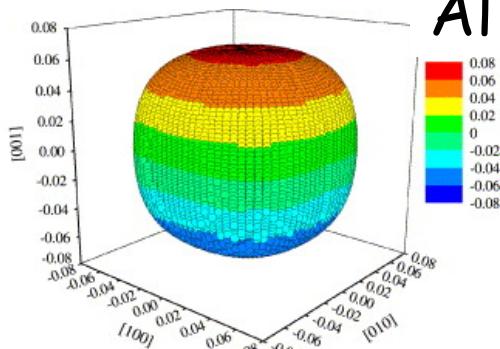
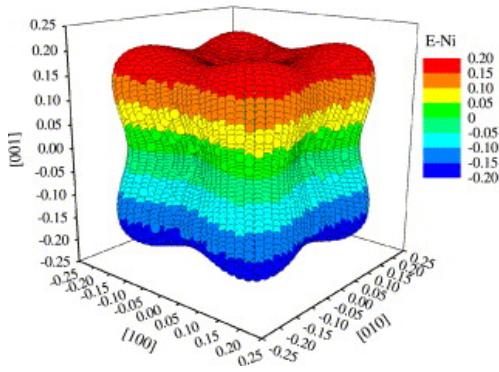
Ag



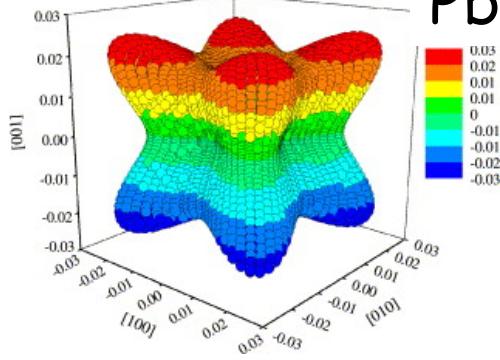
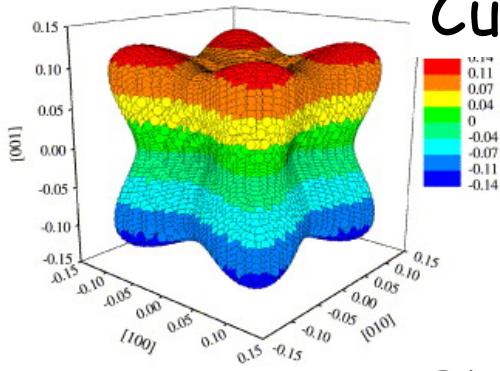
Au



Ni



Cu



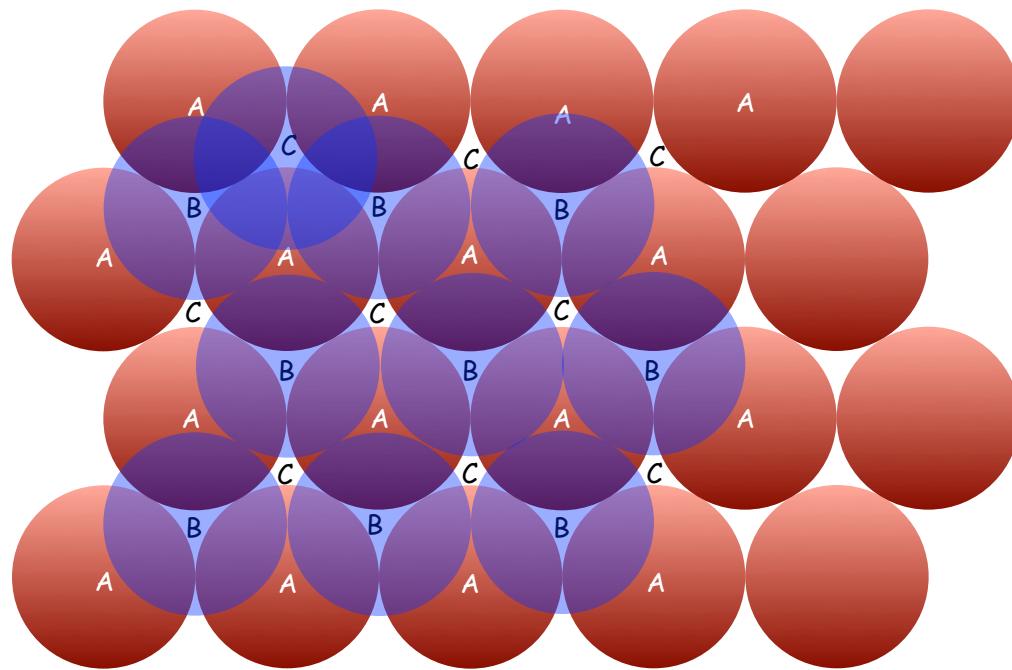
Representation  
surfaces of  
Young's  
modulus of fcc  
metals

Jian-Min Zhang,  
Yan  
Zhang, Ke-Wei Xu and  
Vincent Ji

J Phys. Chem. Solids,  
68 (2007) 503-510

# Close packing of equal hard spheres

3-D packing



First layer A

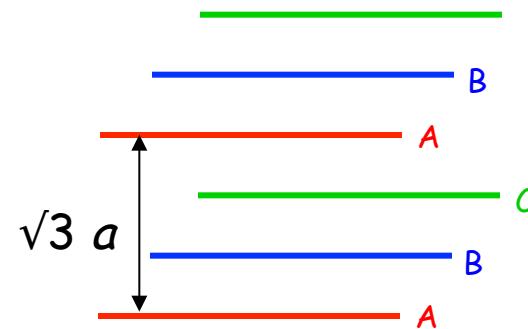
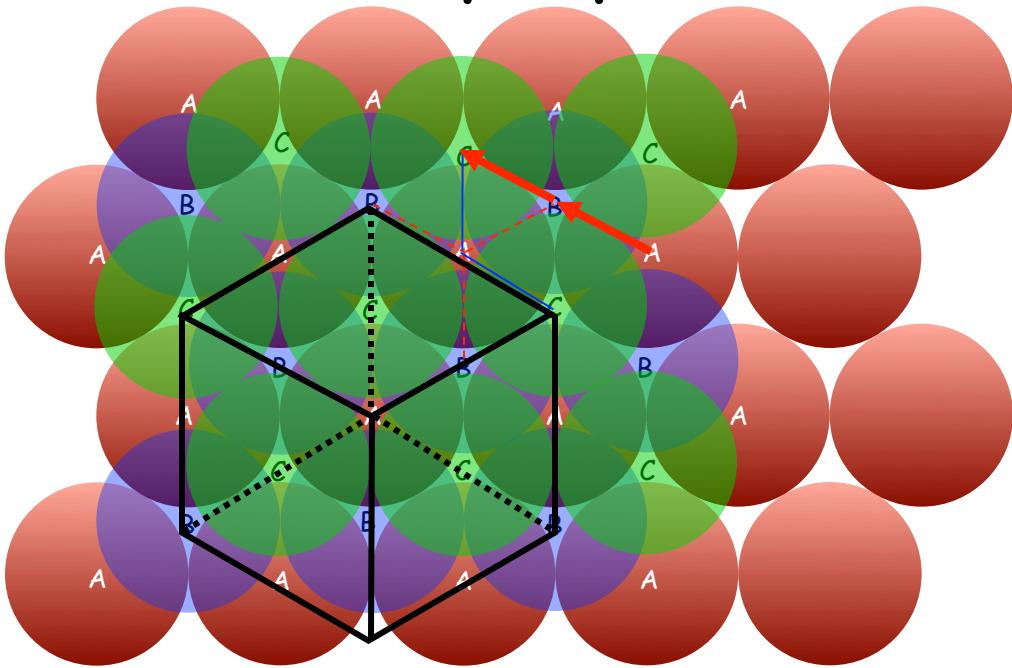
Second layer B

Third layer A or C

Close packed crystals:

...ABABAB... Hexagonal close packed (HCP)  
...ABCABC... Cubic close packed (CCP)

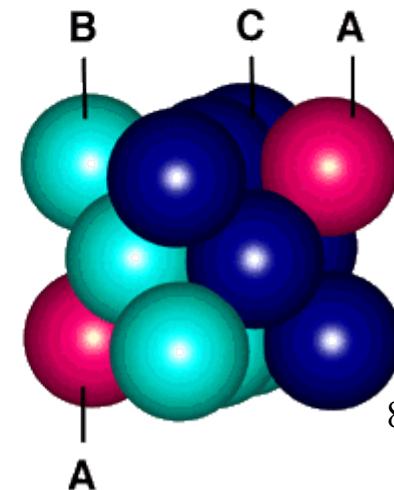
# Geometrical properties of ABCABC stacking



All atoms are equivalent and their centres form a lattice

Motif: single atom 000

ABCABC stacking  
= CCP crystal  
= FCC lattice + single atom motif 000



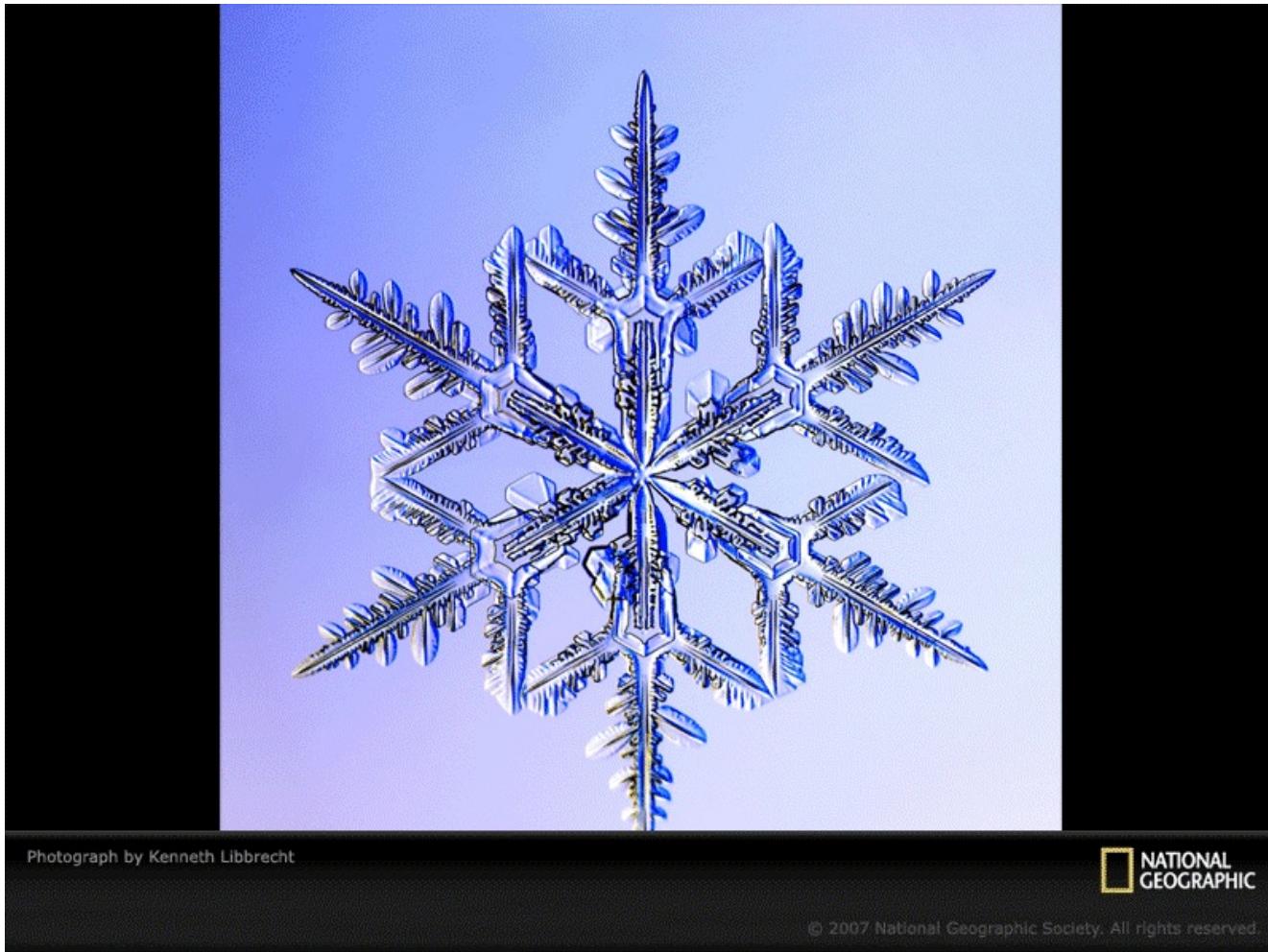
# Orientation Relationships

In solid state phase-transformation, the new crystalline phase has a particular orientation relationship with the parent phase.

When proeutectoid ferrite forms from austenite in steels the following orientation relationship, known as Kurdjumov-Sachs relationship is observed:

$$\begin{aligned}\{110\}_{\alpha} &\parallel \{111\}_{\gamma} \\ <111>_{\alpha} &\parallel <110>_{\gamma}\end{aligned}$$

# Dendrite Growth Directions



FCC

$<100>$

BCC

$<100>$

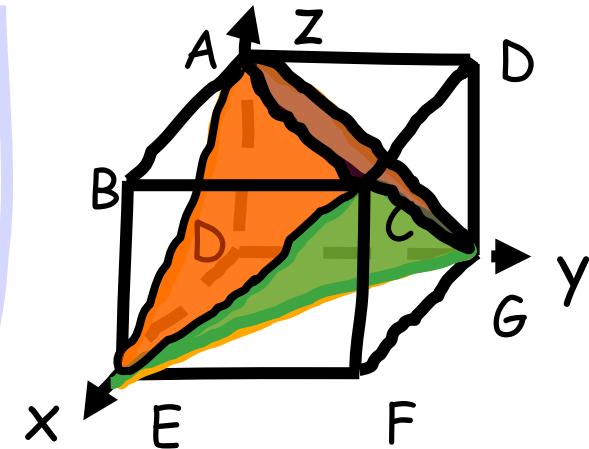
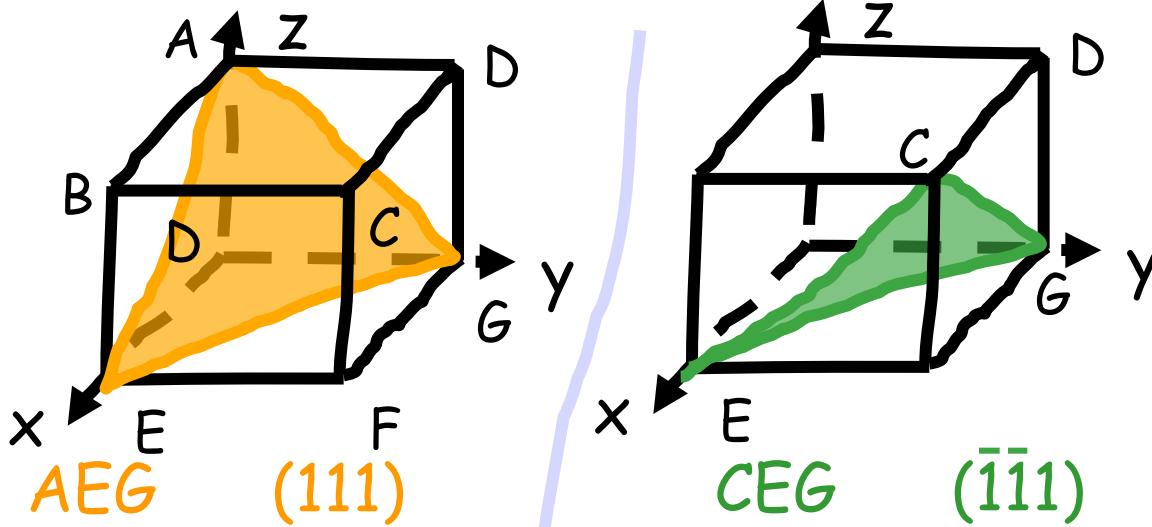
HCP

$<10\bar{1}0>$

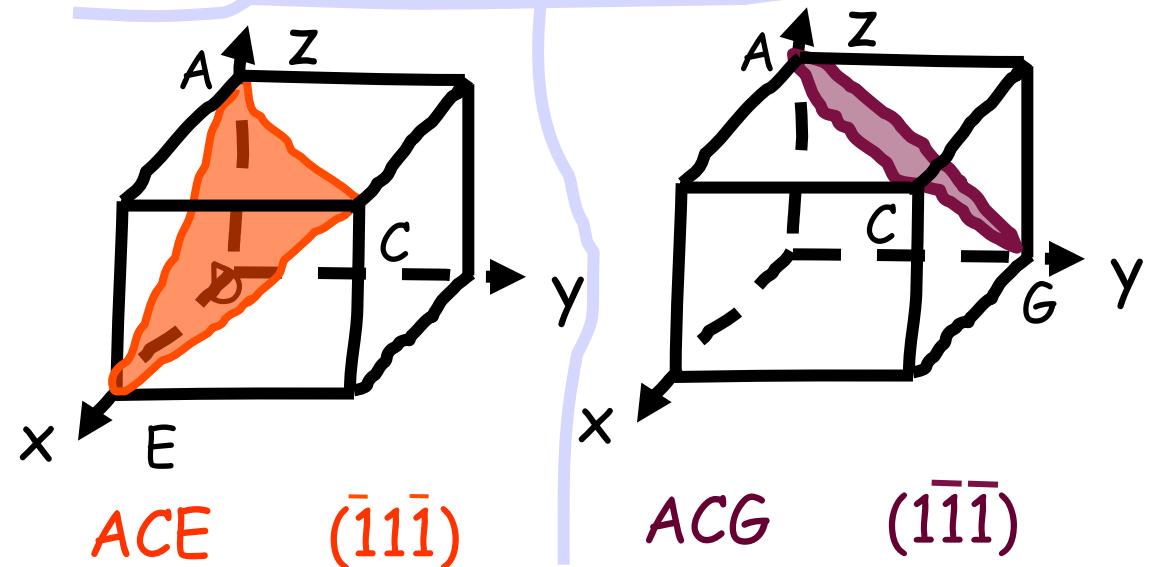
88/  
88

# Slip planes in a ccp crystal

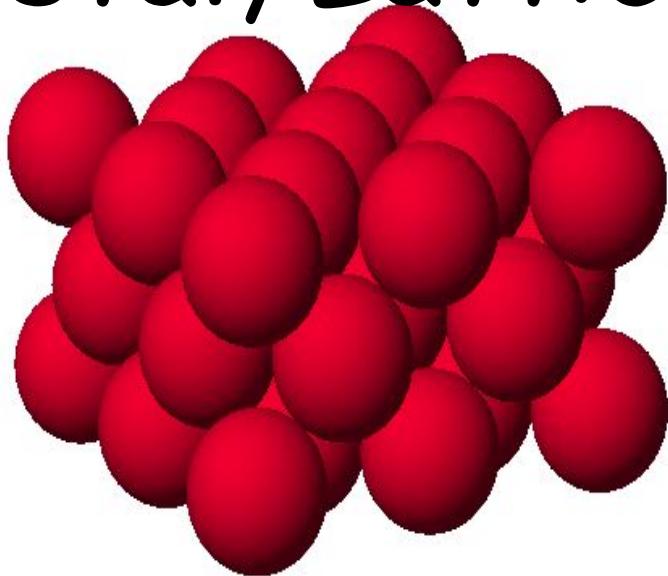
Slip planes in ccp are the close-packed planes



All four slip planes of a ccp crystal:  
 $\{111\}$

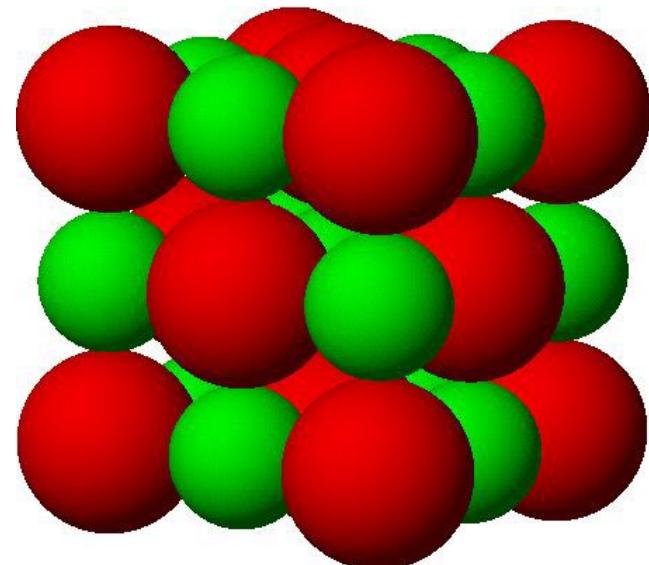


# Crystal, Lattice and Motif



Crystal

Cu Crystal



NaCl Crystal

Lattice

FCC

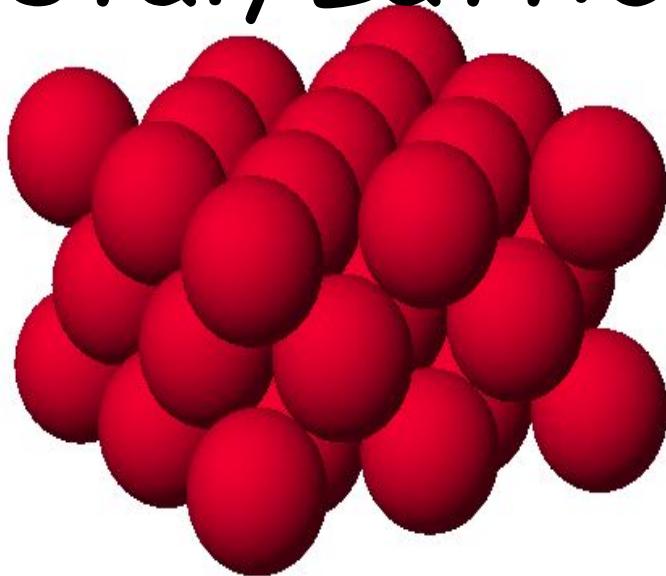
FCC

Motif

$1 \text{ Cu}^+$  ion

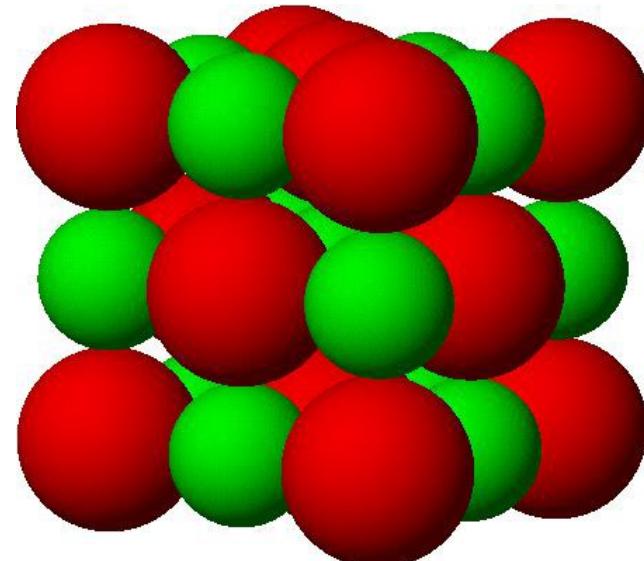
$1 \text{ Na}^+ \text{ ion} + 1 \text{ Cl}^- \text{ ion}$

# Crystal, Lattice and Motif



Crystal

Cu Crystal



NaCl Crystal

Lattice

FCC

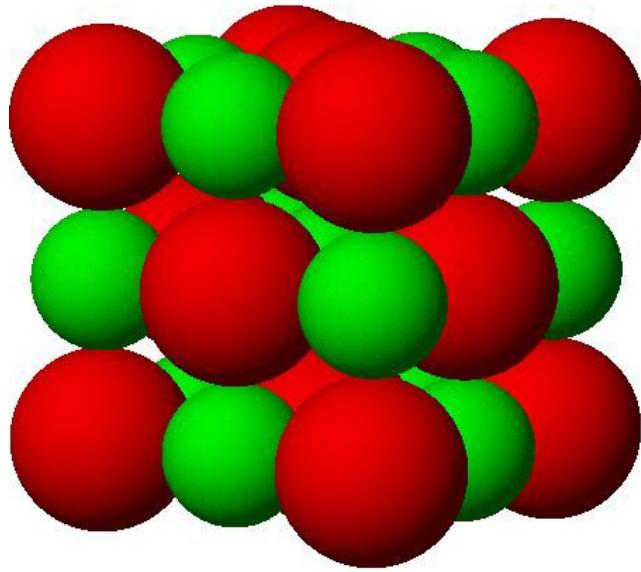
FCC

Motif

$1 \text{ Cu}^+$  ion

$1 \text{ Na}^+ \text{ ion} + 1 \text{ Cl}^- \text{ ion}$

# NaCl Crystal

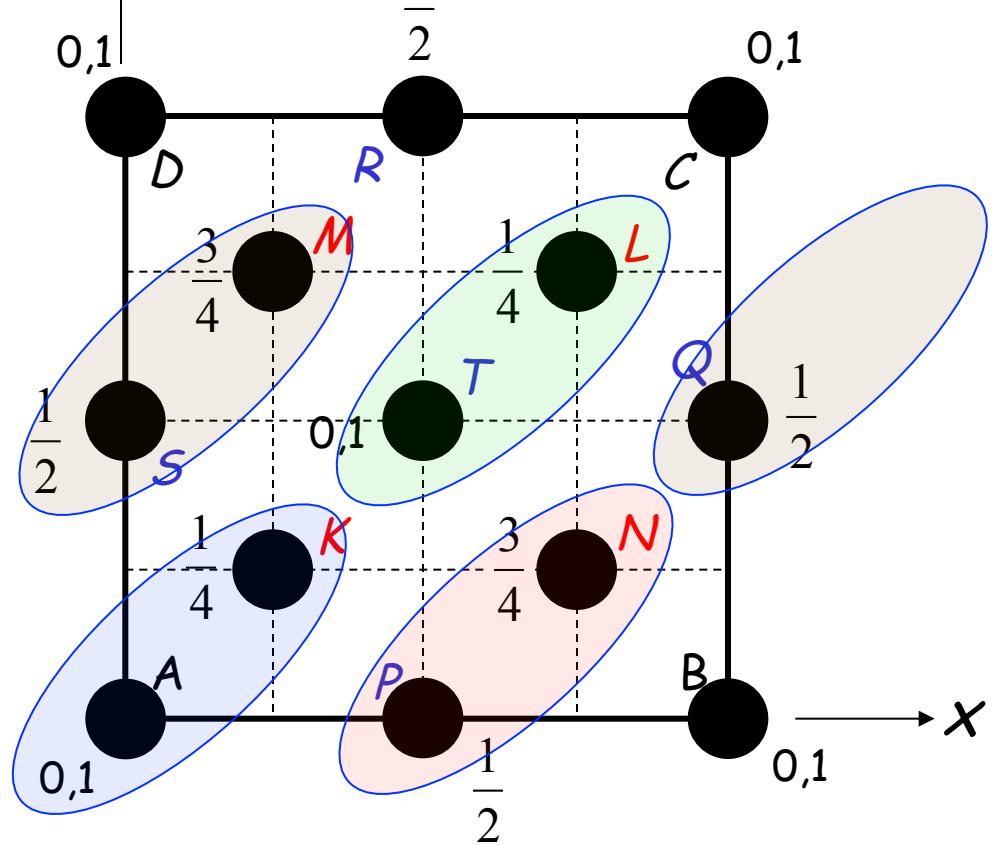
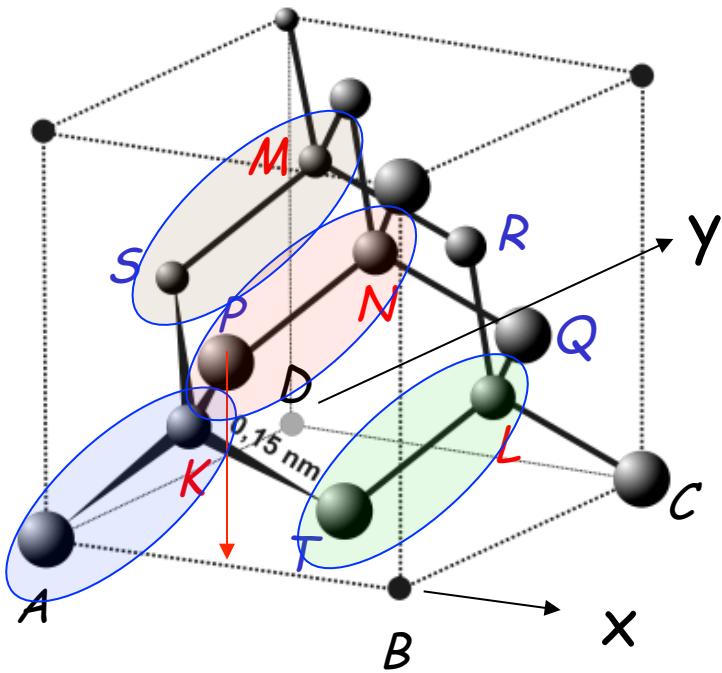


Each  $\text{Na}^+$  is surrounded by six  $\text{Cl}^-$

Each  $\text{Cl}^-$  is surrounded by six  $\text{Na}^+$

Where is the NaCl molecule?

# Diamond Cubic Crystal: Lattice & motif?

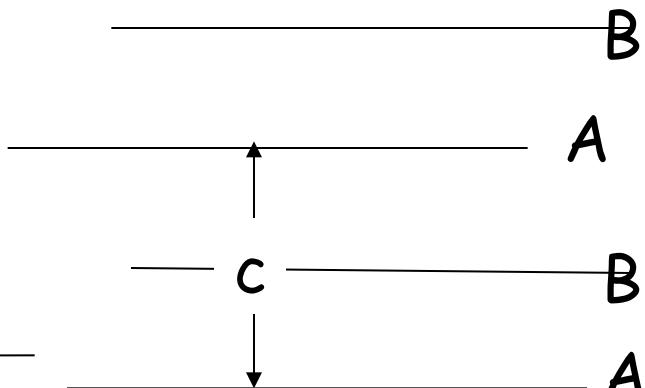
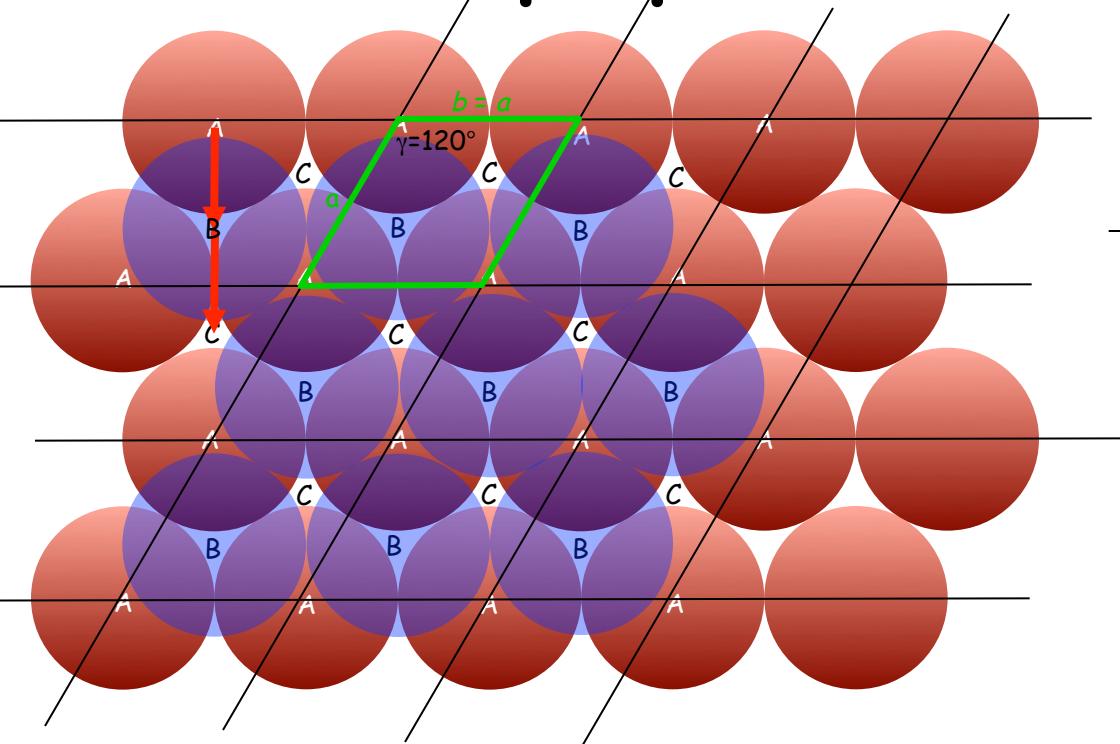


Projection of the unit cell on  
the bottom face of the cube

Diamond Cubic Crystal

= FCC lattice + motif:  $000; \frac{1}{4} \frac{1}{4} \frac{1}{4}$

# Geometrical properties of ABAB stacking



A and B do not have identical neighbours

Either A or B as lattice points, not both

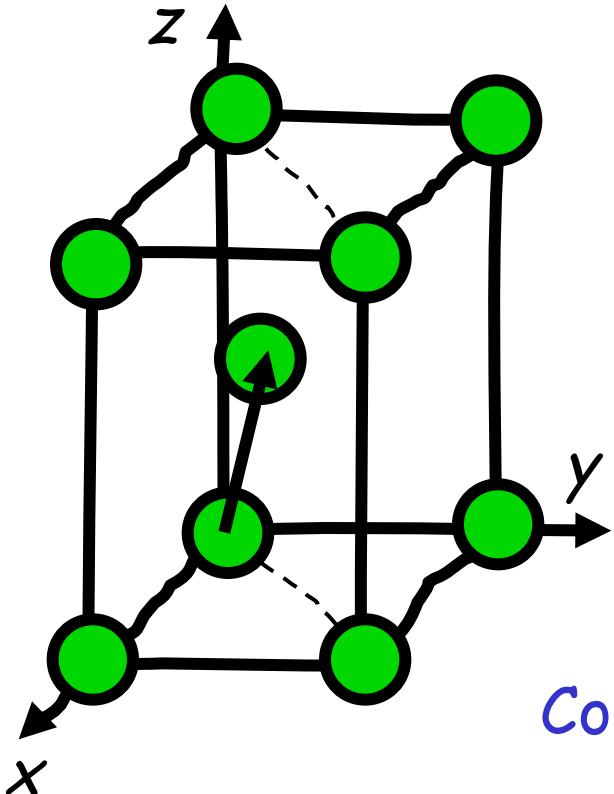
Unit cell: a rhombus based prism with  $a=b\neq c$ ;  $\alpha=\beta=90^\circ$ ,  $\gamma=120^\circ$

The unit cell contains only one lattice point (simple) but two atoms (motif)

ABAB stacking = HCP crystal = Hexagonal P lattice + 2 atom motif

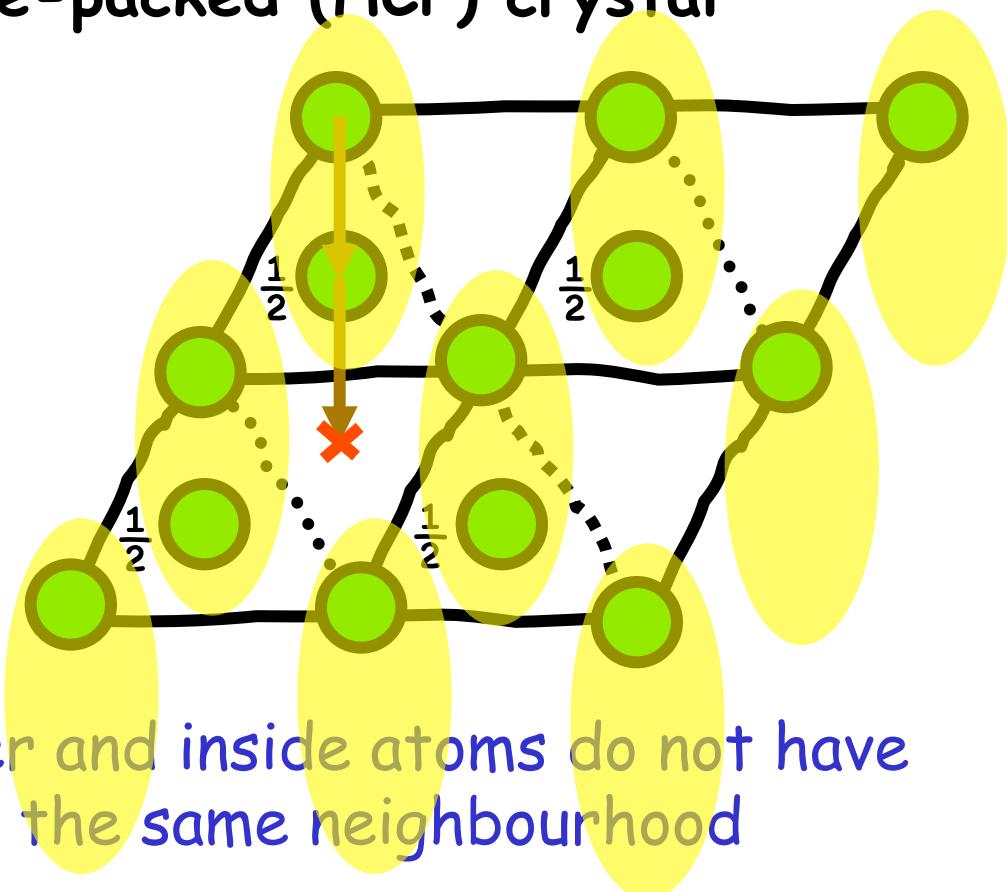
000
2/3 1/3 1/2
1/4 1/4 1/2

# Example: Hexagonal close-packed (HCP) crystal



Lattice: Simple hexagonal

~~hcp lattice~~



Motif: Two atoms:  
 $000; \frac{2}{3} \frac{1}{3} \frac{1}{2}$

~~hcp crystal~~