Introduction to Crystallography

Plastic Deformation in Crystalline Materials

Kamyar Davoudi

Lecture 2

Fall 2015

Crystal

basis

A crystal is formed by periodic repetition of a group of atoms in all directions. That group of atoms is called the **basis**.

- The basis of a crystal can be one or more atoms.
- An ideal crystal consists of infinite repetitions of the basis.

lattice

The infinite array of mathematical points which (describes how the basis is repeated) forms a periodic spatial arrangement is called the **lattice**.

- The lattice looks identical from whichever points you view the array.
- Note that lattice is not a crystal.
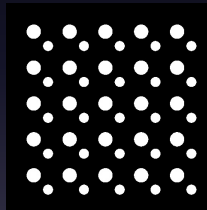
Crystal

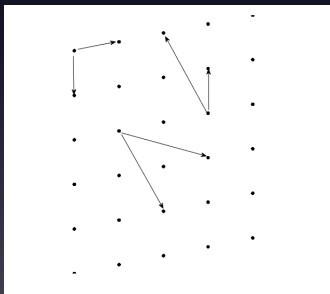Crystal Structure = basis + lattice
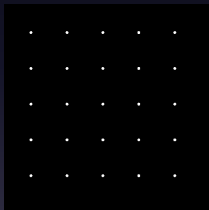
Space lattice   Basis   Crystal Structure

- In three dimensions, the lattice can be identified by three independent vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$ and $\boldsymbol{a}_3$.

- The position of each point $\boldsymbol{R}$ can be written as a linear combination of these vectors,

$$\boldsymbol{R} = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2 + n_3\boldsymbol{a}_3 \tag{1}$$

where n_1, n_2, and n_3 are integers.

- The vectors that can generate or span the lattice are not unique.

Different choices for vectors spanning the lattice

■ The volume of a parallelepiped with axes a_1, a_2 and a_3 is given by $|a_1 \cdot (a_2 \times a_3)|$.
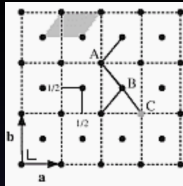
Primitive Cell

Of the vectors satisfying Eq. (1), those that form a parallelepiped with the smallest volume, are called **primitive translation vectors** and the parallelepiped they form is known as the **primitive cell**.
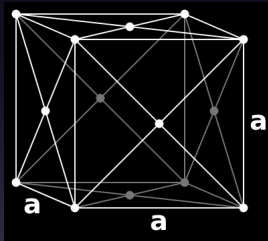
Unit Cell

To better demonstrate the symmetry of the entire lattice, sometimes non-primitive translation vectors are used to specify the lattice. In this case the parallelepiped is called the **unit cell**.
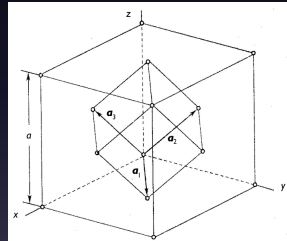
■ The unit cell may or may not be identical to the primitive cell.

Primitive cell is shown in gray [De Graef & McHenry, Structure of Materials, Cambridge University Press]

Unit cell of a face-centered cubic structure

Primitive unit cell of a face-centered cubic structure. As drawn, the primitive translation vectors are

$$\boldsymbol{a}_1 = \frac{a}{2}(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}}) \quad \boldsymbol{a}_2 = \frac{a}{2}(\hat{\boldsymbol{y}} + \hat{\boldsymbol{z}}) \quad \boldsymbol{a}_3 = \frac{a}{2}(\hat{\boldsymbol{x}} + \hat{\boldsymbol{z}})$$
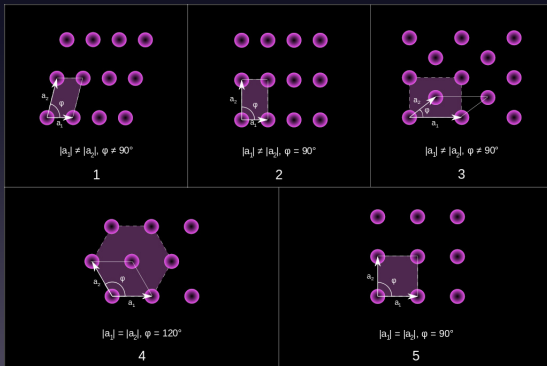
[Kittel, Introduction to Solid State Physics, Wiley]

Lattice Parameters

The length of axes of the unit cell (called **lattice constants** *a*, *b*, and *c*) and the angle between the axes (α, β and γ) specify the unit cell. The lattice constants and the three angles between them are termed **lattice parameters**.
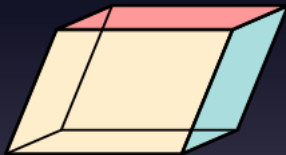
Bravais lattices

- Auguste Bravais, a French physicist, identified 14 distinct lattices in three dimensions.

- There are 5 Bravais lattice in two dimensions (shown below)

- In crystallography, all lattices are traditionally called **Bravais lattices** or **translation lattices**.

$|a_2| \neq |a_1|, \varphi \neq 90°$ 1	$|a_2| \neq |a_1|, \varphi = 90°$ 2	$|a_2| \neq |a_1|, \varphi \neq 90°$ 3

$|a_1| = |a_2|, \varphi = 120°$
4

$|a_1| = |a_2|, \varphi = 90°$
5

The five fundamental 2D Bravais lattices: (1) oblique, (2) rectangular, (3) centered rectangular, (4) hexagonal (rhombic), and (5) square
[ref]

3D Bravais lattices

▸ Wikipedia: Bravais Lattice
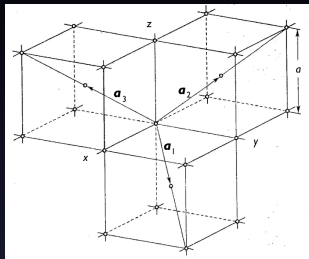
also

▸ Bravais Lattice

Packing Fraction

- We try to pack N hard spheres (cannot deform)
- The total volume of the spheres is

$$V_s = N\frac{4}{3}\pi R^3$$

- The volume these spheres occupy $V > V_S$ (there are spacing)

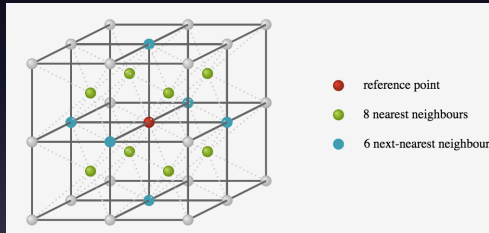$$\text{Packing Fraction} = \frac{N\frac{4}{3}\pi R^3}{V}$$

Body Centered Cubic (BCC)

the primitive translation vectors are:

$$\boldsymbol{a}_1 = \frac{a}{2}(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}} - \hat{\boldsymbol{z}})$$

$$\boldsymbol{a}_2 = \frac{a}{2}(-\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}} + \hat{\boldsymbol{z}})$$

$$\boldsymbol{a}_3 = \frac{a}{2}(\hat{\boldsymbol{x}} - \hat{\boldsymbol{y}} + \hat{\boldsymbol{z}})$$

- The primitive unit cell is a rhombohedron of edge $a\frac{\sqrt{3}}{2}$
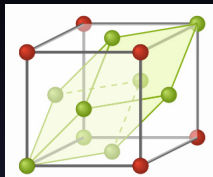- The angle between adjacent edges is $109°28'$

reference point
8 nearest neighbours
6 next-nearest neighbour

[http://www.physics-in-a-nutshell.com/article/12]

- Packing fraction $\frac{1}{8}\pi\sqrt{3} \approx 0.680$

Some Elements with BCC structure

Barium	Ba	Chromium	Cr
Caesium	Cs	α–Iron	α–Fe
Potassium	K	Lithium	Li
Molybdenum	Mo	Sodium	Na
Niobium	Nb	Rubidium	Rb
Tantalum	Ta	Titanium	Ti
Vanadium	V	Tungsten	W

Face Centered Cubic (FCC)

the primitive translation vectors are:

$$\boldsymbol{a}_1 = \frac{a}{2}(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}})$$

$$\boldsymbol{a}_2 = \frac{a}{2}(\hat{\boldsymbol{y}} + \hat{\boldsymbol{z}})$$

$$\boldsymbol{a}_3 = \frac{a}{2}(\hat{\boldsymbol{x}} + \hat{\boldsymbol{z}})$$

■ The angle between adjacent edges is 60○

● reference point

● ● ● 12 nearest neighbours

● 6 next-nearest neighbours
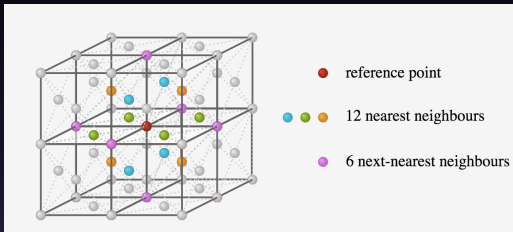
■ Packing fraction $\frac{1}{6}\pi\sqrt{2} \approx 0.740$

■ Some elements with fcc structure: Ar, Ag, Al, Au, Ca, Ce, $\beta-$Co, Cu, Ir, Kr, La, Ne, Ni, Pb, Pd, Pr, Pt, $\delta-$Pu, Rh, Sc, Sr, Th, Xe, Yb

[Figures from http://www.physics-in-a-nutshell.com/article/11]

Characteristics of Cubic structure

|	simple cubic	b.c.c	f.c.c.
volume of conventional cell	a^3	a^3	a^3
no. of lattice points per cell	1	2	4
no. of nearest neighbors (coordination number)	6	8	12
no. of 2nd nearest neighbors	12	6	6
nearest neighbor distance	a	$\frac{\sqrt{3}}{2}a \approx 0.866a$	$\frac{a}{\sqrt{2}} \approx 0.707a$
2nd nearest neighbor distance	$a\sqrt{2}$	a	a
packing fraction	$\pi/6 \approx 0.52$	$\pi\sqrt{3}/8 \approx 0.68$	$\pi\sqrt{2}/6 \approx 0.74$

[Kittel, Introduction to Solid State Physics]

Phase Diagram of Pure Iron
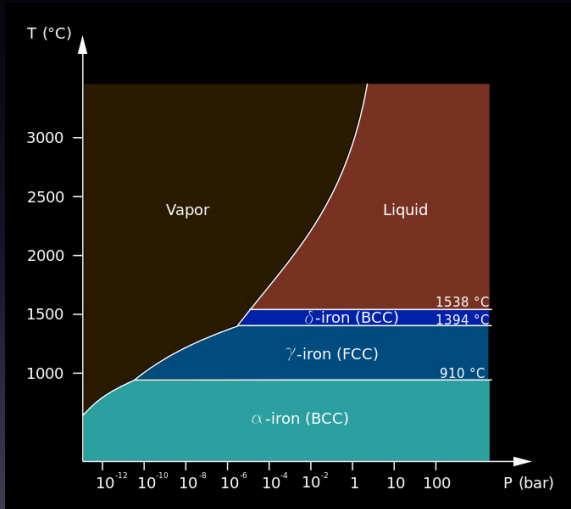
Hexagonal Close Packed (HCP) Structure
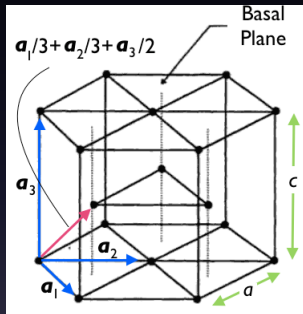
- It can be viewed as two nested simple hexagonal Bravais lattice shifted by $a_1/3 + a_2/3 + a_3/2$.

  where

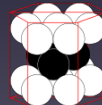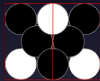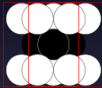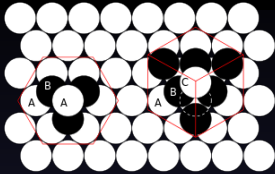 $$a_1 = a\hat{x}, \; a_2 = \frac{a}{2}\hat{x} + \frac{a\sqrt{3}}{2}\hat{y}, \quad a_3 = c\hat{z}$$

- 30 elements crystallize in hcp form
- Not a Bravais lattice

Close Packed Structures

- In this figure, the left structure is hcp and the right is fcc

- volume fraction = 0.74

- number of nearest neighbors (coordination number) is 12 for both hcp and fcc structures

- Although a hexagonal close-packing of equal atoms is only obtained if $c/a = \sqrt{8/3} \approx 1.63$, the term hcp is used for any structure described in the previous slide.

[figure from
https://en.wikipedia.org/wiki/Close-packing_of_equal_spheres]

hcp   fcc

Elements with hcp structures

Element	c/a	Element	c/a
Ideal	1.63		
Be	1.56	Cd	1.89
Ce	1.63	α-Co	1.62
Dy	1.57	Er	1.57
Gd	1.59	He (2K)	1.63
Hf	1.58	Ho	1.57
La	1.62	Lu	1.59
Mg	1.62	Nd	1.61
Os	1.58	Pr	1.61
Re	1.62	Ru	1.59
Tb	1.58	Ti	1.59
Tl	1.60	Tm	1.57
Y	1.57	Zn	1.59

[adapted from Ashcroft, Mermin, Solid State Physics]

Diamond Structure

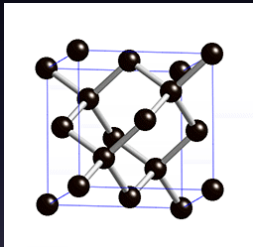- it is the structure of carbon in a diamond crystal
- It can be viewed as two interpenetrating fcc lattices displaced by $\frac{a}{4}(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}})$
- or it can be imagined as an fcc with two point basis $\mathbf{0}$ and $\frac{a}{4}(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}})$.
- Coordination number is 4
- Packing fraction is $\frac{\sqrt{3}}{16}\pi \approx 0.34$

fcc structure   two-atomic basis

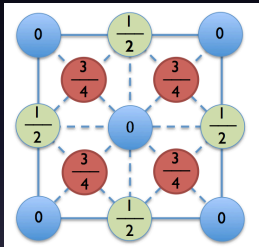[http://www.physics-in-a-nutshell.com/article/13]
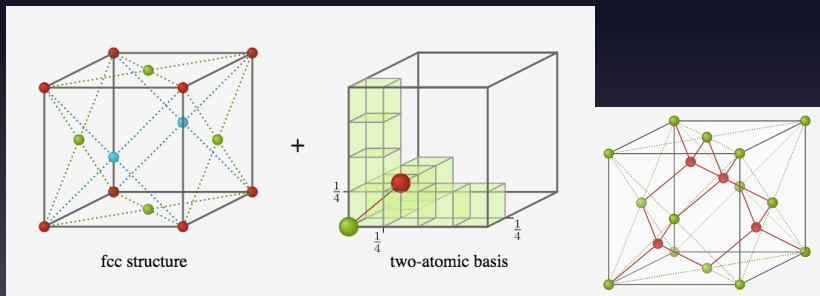
Diamond Structure

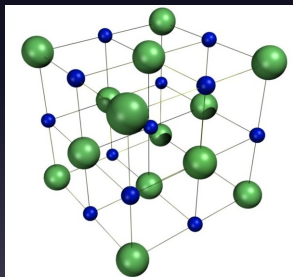(a)   (b)

(a) tetrahedral bond in a diamond structure (b) diamond structure projected on a cube face. Fractions denote the height above the base in units of a

Elements with diamond structure: C (diamond), Si, Ge, α-Sn (grey)

Sodium Chloride Structure

■ Na^+ and Cl^- ions are placed on alternate points of a simple cubic structure

■ The lattice is fcc; the basis consists of Na^+ and Cl^-

[NaCl structure]

Some compounds with sodium chloride structure

LiF	LiCl	LiBr	LiI
NaF	NaCl	NaBr	NaI
RbF	RbCl	RbBr	RbI
CsF			
AgF	AgCl	AgBr	
MgO	MgS	MgSe	
CaO	CaS	CaSe	CaTe
SrO	SrS	SrSe	SrTe
BaO	BaS	BaSe	BaTe

[Adapted from Ashcroft, Mermin, Solid State Physics]

Cesium Chloride Structure

■ Cs^+ and Cl^- ions are placed at **0** and body center position $\frac{a}{2}(\hat{\boldsymbol{x}}+\hat{\boldsymbol{y}}+\hat{\boldsymbol{y}})$, respectively.

■ The lattice is simple cubic; the basis consists of Cs^+ and Cl^-
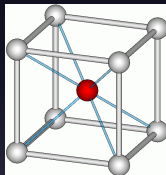
CsCl structure

■ Some compounds with the cesium chloride structure:
  CsCl   CsBr   CsI
  TlCl   TlBr   TlI
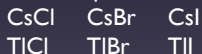
# Miller Indices for Directions in Cubic Structure

- It is often required to specify certain directions and planes in crystals. To this end, we use *Miller indices*.

- $[hkl]$ represents the direction vector $h\hat{x} + k\hat{y} + l\hat{z}$ of a line passing through the origin.

- These integers h, k and l must be the smallest numbers that will give the desired direction. i.e. we write $[111]$ not $[222]$.

- If a component is negative, it is conventionally specified by placing a bar over the corresponding index. For example, we write $[1\bar{1}1]$ instead of $[1-11]$.

- Coordinates in angle brackets such as $\langle 123 \rangle$ denote a family of directions that are equivalent due to symmetry operations, such as $[123]$, $[132]$, $[321]$, $[\bar{1}23]$, $[\bar{1}\bar{2}3]$, etc.
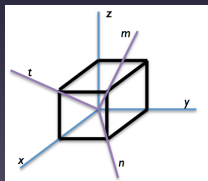
$[111]$, $[101]$, and $[110]$ describe directions m, t, and n, respectively.

Miller Indices for Planes in Cubic Structure

■ A crystallographic plane is denoted by the Miller indices of the direction normal to the plane, but instead of brackets we use parenthesis, i.e. (*hkl*)
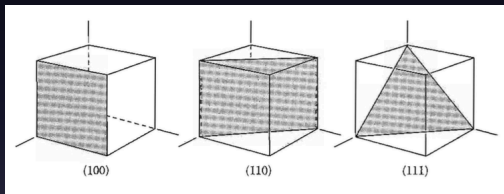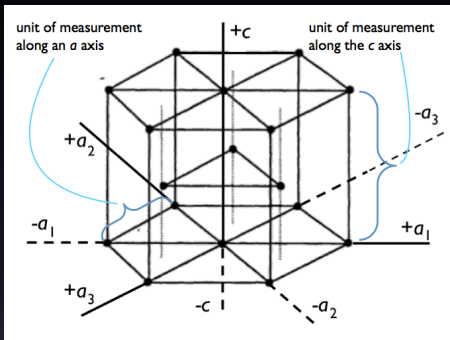

[Kittel, Introduction to Solid State Physics]

■ ``Coordinates in curly brackets or braces such as {100} denote a family of plane normals that are equivalent due to symmetry operations, much the way angle brackets denote a family of directions."

Miller Indices for hcp

unit of measurement along an *a* axis

unit of measurement along the *c* axis

$+c$

$-a_3$

$+a_2$

$-a_1$

$+a_1$

$+a_3$

$-c$

$-a_2$

- Directions along axes a_1, a_2 and a_3 are of type $\langle \bar{1}2\bar{1}0 \rangle$.

- (*hkil*) is a plane the normal direction of which is [*hkil*].

a_3

a_2

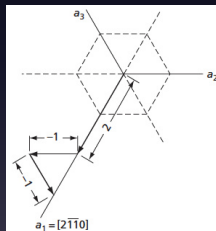$a_1 = [2\bar{1}\bar{1}0]$

FIG. 1.18 Determination of indices of a digonal axis of Type I—[$2\bar{1}\,\bar{1}0$]
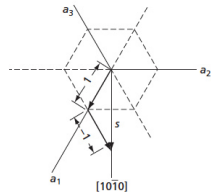
a_3

a_2

a_1

s

$[10\bar{1}0]$

FIG. 1.19 Determination of indices of a digonal axis of Type II—[$10\bar{1}0$]

Reed, Physical Metallurgy Principles]

- Miller indices contains 4 digits instead of 3 digits

- [*hkil*] means:

$$\{\alpha(h a_1 + k a_2 + i a_3 + l c) : \alpha \in \mathbb{R}\}$$

and

$$h + k + i = 0$$

Further Reading

■ Ashcroft, N.W., Mermin, N.D., *Solid State Physics*, Harcourt College Publishers, 1976.

■ De Graef, M., McHenry, M.E., *Structure of Materials*, Cambridge University Press, 2007.

■ Kittel, C., *Introduction to Solid State Physics*, 8th ed., Wiley, 2004.