Analytical Methods for Materials

Lesson 10
Crystallography and Crystal Structures, Part 2

Suggested Reading

- Chapters 2 and 6 in Waseda

Symmetry Operators

- All motions that allow a pattern to be transformed from an initial position to a final position such that the initial and final patterns are indistinguishable.

1. Translation*
2. Reflection
3. Rotation
4. Inversion (center of symmetry)

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5. Roto-inversion (inversion axis)
6. Roto-reflection
7. Glide (translation + reflection)
8. Screw (rotation + translation)

These are compound symmetry operators (combinations of 1-4)

Remember

- Bravais lattices are either:
  - primitive (i.e., simple)
  - non-primitive (i.e., body-, face-, or base- centered)
- Bravais lattices have specific lattice point locations.
- To produce a crystal, we will place an identical motif on each lattice point.
- Some people call the motif the basis.

Allowed Locations of Lattice Points

- Primitive
  - Lattice site at origin [i.e., at (0, 0, 0)]
- Body centering
  - Add a lattice site to the center of the primitive unit cell. [i.e., at (1/2,1/2,1/2)]
- Face centering
  - Add a lattice site to the center of all faces of the primitive cell.
    [i.e., at (1/2,1/2,0), (1/2,0,1/2), and (0,1/2,1/2)]
- Base centering
  - Add a lattice site to the center of only one face of the primitive cell.
  - [i.e., at (1/2,1/2,0) or (1/2,0,1/2) or (0,1/2,1/2)]

Table 2.1 Summary of seven crystal systems and Bravais lattices

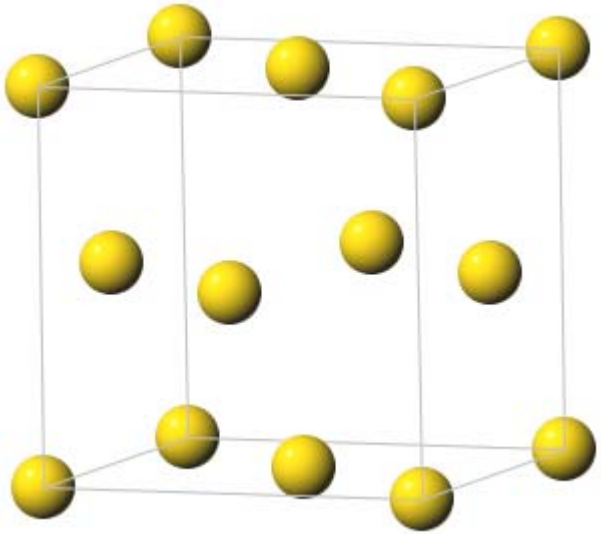
System	Axial lengths and angles	Bravais lattice	Lattice symbol
Cubic	Three equal axes at right angles $a = b = c, \alpha = \beta = \gamma = 90°$	Simple Body-centered Face-centered	P I F
Tetragonal	Three axes at right angles, two equals $a = b \neq c, \alpha = \beta = \gamma = 90°$	Simple Body-centered	P I
Orthorhombic	Three unequal axes at right angles $a \neq b \neq c, \alpha = \beta = \gamma = 90°$	Simple Body-centered Base-centered Face-centered	P I C F
Trigonal*	Three equal axes, equally inclined $a = b = c, \alpha = \beta = \gamma \neq 90°$	Simple	R
Hexagonal	Two equal coplanar axes at, 120° third axis at right angles $a = b \neq c, \alpha = \beta = 90°, \gamma = 120°$	Simple	P
Monoclinic	Three unequal axes, one pair not at right angles $a \neq b \neq c$, $\alpha \neq \gamma = 90° \neq \beta$	Simple Base-centered	P C
Triclinic	Three unequal axes, unequally inclined and none at right angles $a \neq b \neq c, \alpha \neq \beta \neq \gamma \neq 90°$	Simple	P

*Also called rhombohedral.

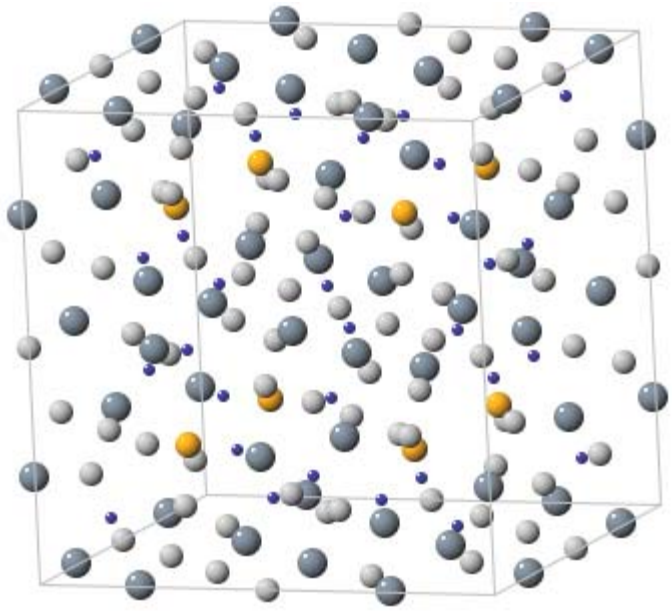
Remember

- In a Bravais lattice, the objects making up the motif/basis will have their own coordinates.

- This is important from the standpoint of diffraction and diffraction analysis.



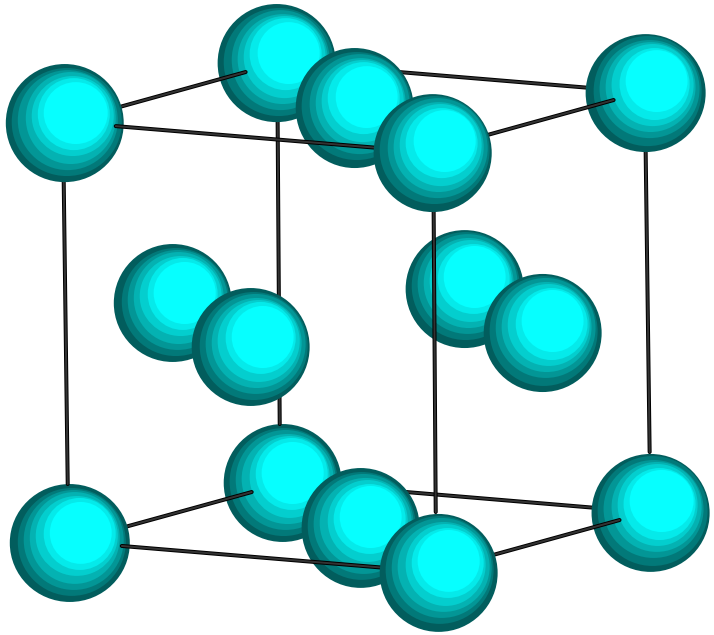
Au
cF4 ; A1 ; SG #225 ; Fm3m
4 atoms/UC



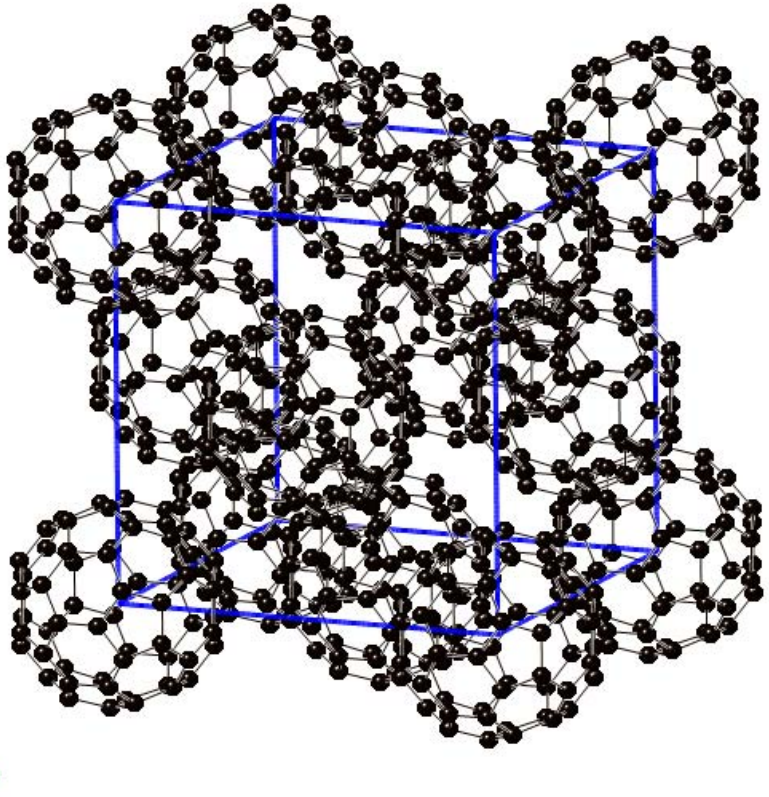
$Cr_{23}C_6$
cF116 ; $D8_4$; SG #225 ; Fm3m
116 atoms/UC

Both of these crystals are FCC!
HOW?

Examples of crystals with FCC Bravais lattices



Cu
Fm3m



Buckminsterfullerene
Fm3m

The Basis or Motif

- By definition the **basis/motif** is the **list of atoms associated with** each *lattice point** along with their fractional coordinates relative to each lattice point. Also…

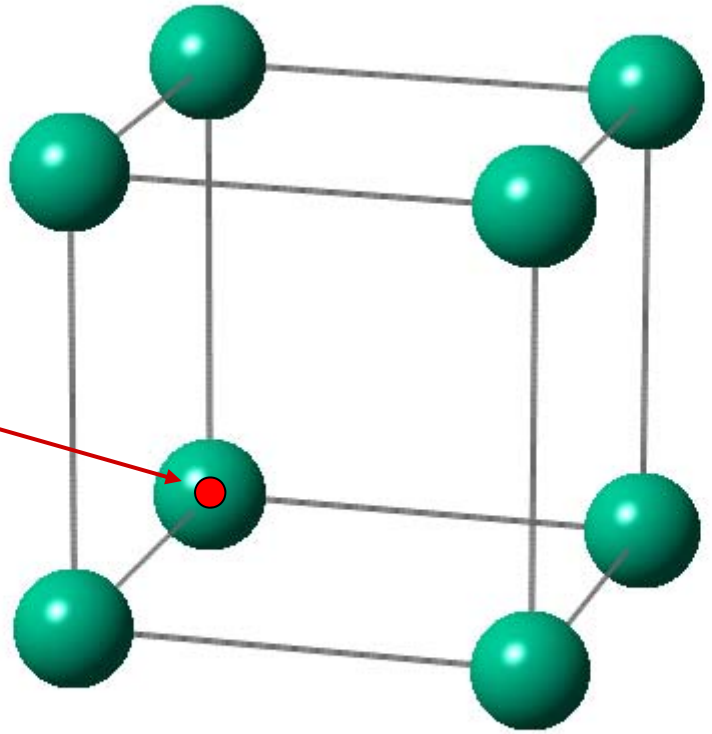
$$Basis, B = \frac{(\#\ \text{atoms / unit cell})}{(\#\ \text{lattice points / unit cell})}$$

- The number of atom positions in the basis is often different than the number of atoms/unit cell.
- This is not a lattice or number of lattice points! In a basis, side occupancy is allowed!

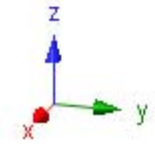
Simple Cubic Lattice

WHAT IS THE BASIS?

$a = b = c$



Required Lattice Points (0,0,0)



1 atom must be defined
1 equivalent lattice points in SC
1 atom on each lattice point

For a Simple Cubic *crystal*

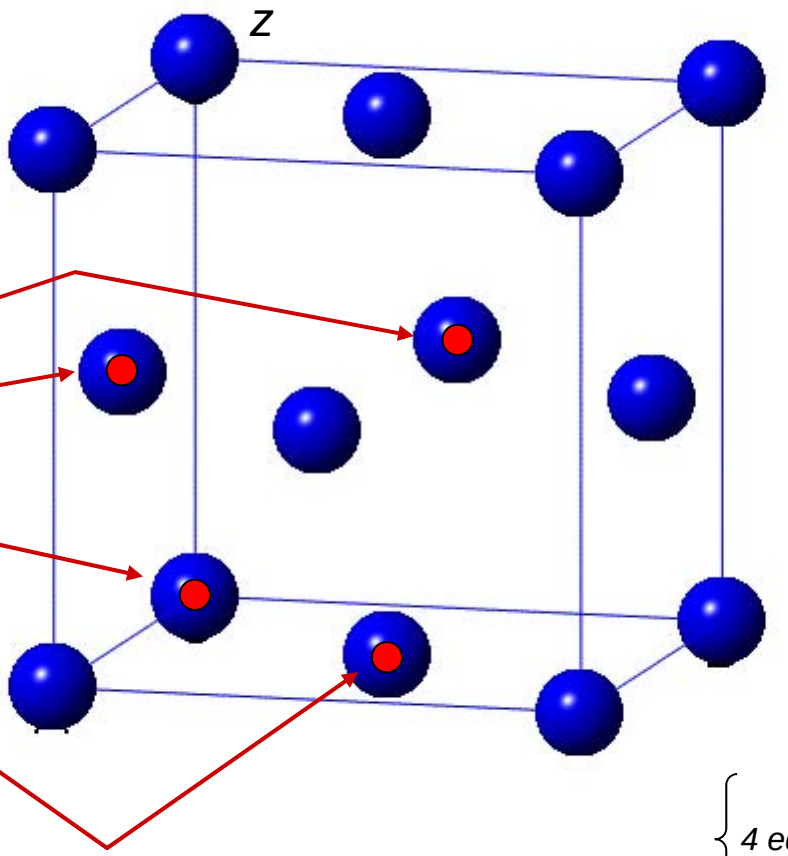
Place single atom at 0,0,0

$$B = \frac{\left(0 + \frac{0}{2} + \frac{8}{8}\right)}{1} = \frac{1}{1} = 1 \ \frac{\text{Atom}}{\text{SC lattice point}}$$

This is a primitive lattice (Simple Cubic)

Face-centered Cubic Lattice

WHAT IS THE BASIS?



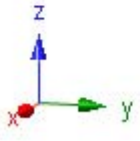
Required Lattice Points

(0,1/2,1/2)

(1/2,0,1/2)

(0,0,0)

(1/2,1/2,0)



4 atoms must be defined
4 equivalent lattice points in FCC
1 atom on each lattice point

For a Face-centered Cubic *crystal*

Place single atoms on the four required lattice points

$$B = \frac{\left(0 + \frac{6}{2} + \frac{8}{8}\right)}{4} = \frac{4}{4} = 1 \frac{\text{Atoms}}{\text{FCC lattice points}}$$

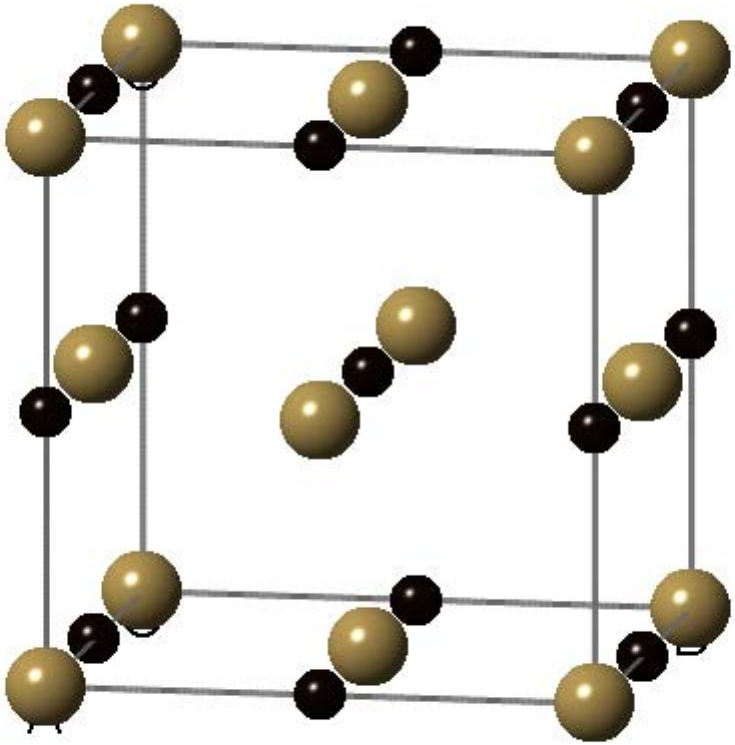
This is a non-primitive lattice (FCC)

Tantalum Carbide

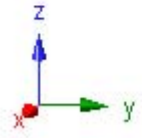
WHAT IS THE BASIS?

Tantalum

Carbon



$a = b = c$



8 atoms must be defined
4 equivalent lattice points in FCC
2 atoms on each lattice point

For this *crystal*

$$B = \frac{\left(1 + \frac{6}{2} + \frac{12}{4} + \frac{8}{8}\right)}{4} = \frac{8}{4} = 2 \frac{\text{Atoms}}{\text{FCC lattice points}}$$

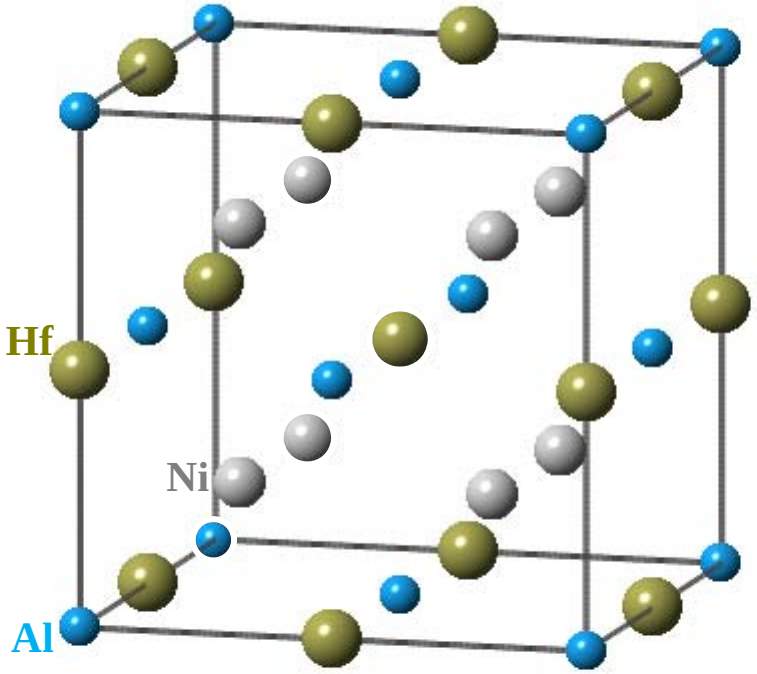
Ni_2AlHf

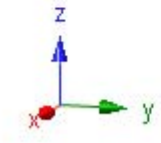
WHAT IS THE BASIS?

$a = b = c$

Aluminum

Nickel





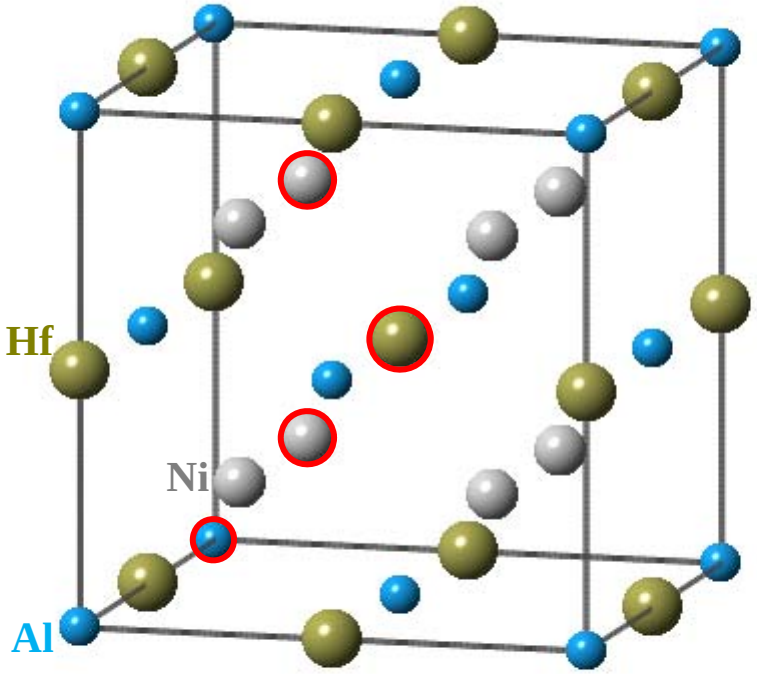
Hafnium

$B =$

Ni_2AlHf

WHAT IS THE BASIS?

$a = b = c$



Aluminum

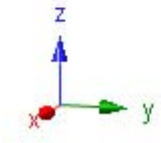
(0,0,0) ←
(0, ½, ½)
(½,0,½)
(½, ½,0)

Nickel

(¼,¼,¼) ←
(¾,¾,¾)
(¼,¾,¾)
(¾,¼,¾)
(¾,¾,¼)
(¾,¼,¼)
(¼,¾,¼)
(¼,¼,¾) ←

Hafnium

(½,½,½) ←
(½,0,0)
(0,½,0)
(0,0,½)



16 atoms must be defined
4 equivalent lattice points in FCC
4 atoms on each lattice point

$$B = \frac{\left(9 + \frac{6}{2} + \frac{12}{4} + \frac{8}{8}\right)}{4} = \frac{16}{4} = 4 \frac{\text{Atoms}}{\text{FCC lattice point}}$$

Important!

The fraction of atoms in the basis must match the chemical formula of the compound.

SIMPLE CUBIC LATTICE

LATTICE PTS. = 1

MOTIF = 2 atoms

blue atom at (0,0,0)

Grey atom at (½,½,½)

CsCl crystal structure