



# 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  $(0, 1/2, 1/2)$ ]

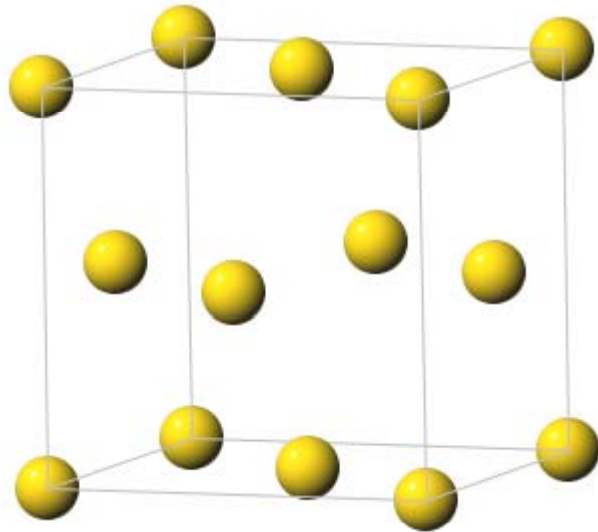
**Table 2.1** Summary of seven crystal systems and Bravais lattices

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

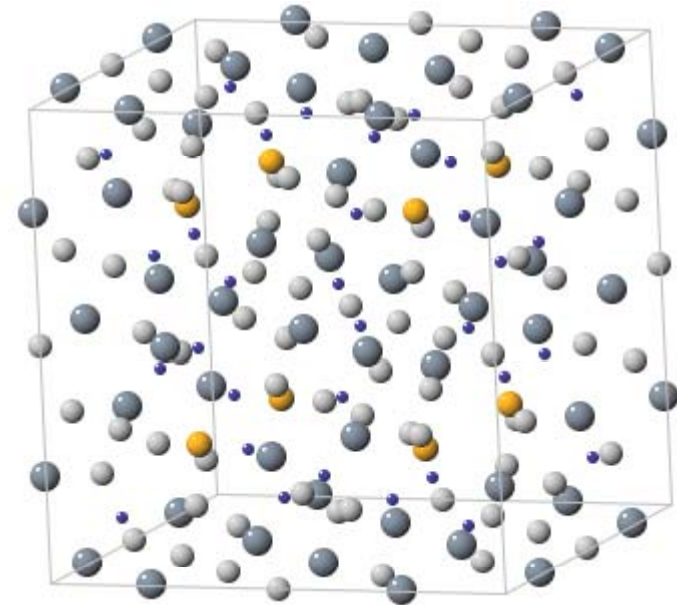
\*Also called rhombohedral.

# 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<sub>23</sub>C<sub>6</sub>**  
**cF116 ; D<sub>8</sub><sub>4</sub> ; SG #225 ; Fm3m**  
 116 atoms/UC

Both of these crystals are FCC!  
**HOW?**

# 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...

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

- 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, site occupancy is allowed!

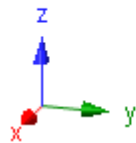
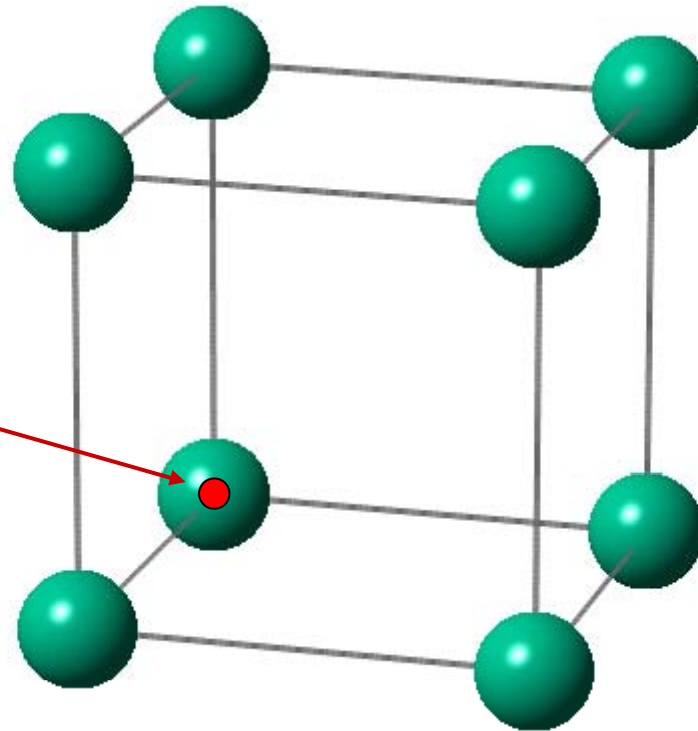
# Simple Cubic Lattice

## WHAT IS THE BASIS?

$$a = b = c$$



Required  
Lattice Points  
(0,0,0)



For a Simple Cubic  
*crystal*

Place single atom at 0,0,0

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

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



This is a primitive lattice  
(Simple Cubic)

# Face-centered Cubic Lattice

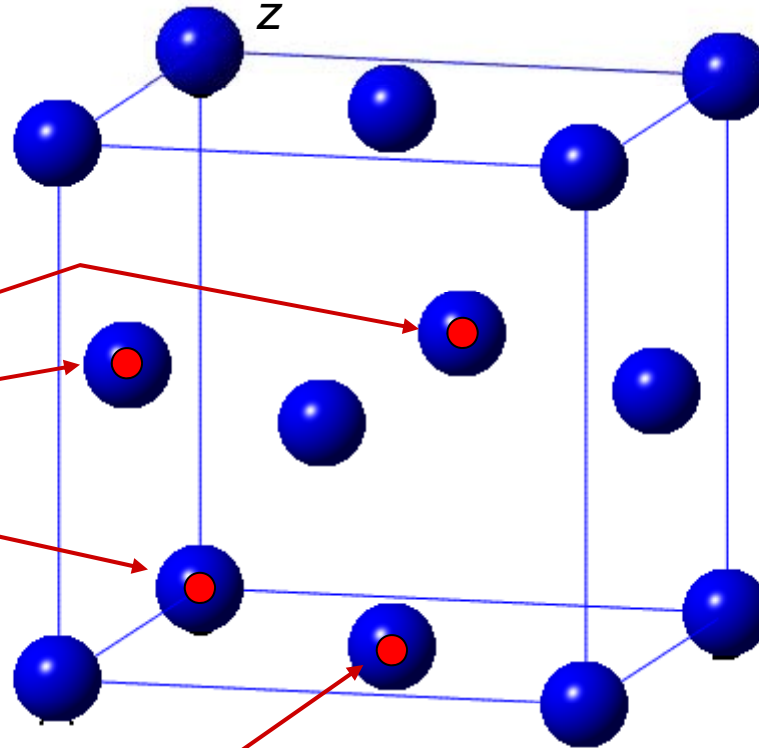
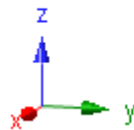
## WHAT IS THE BASIS?



$$a = b = c$$

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)

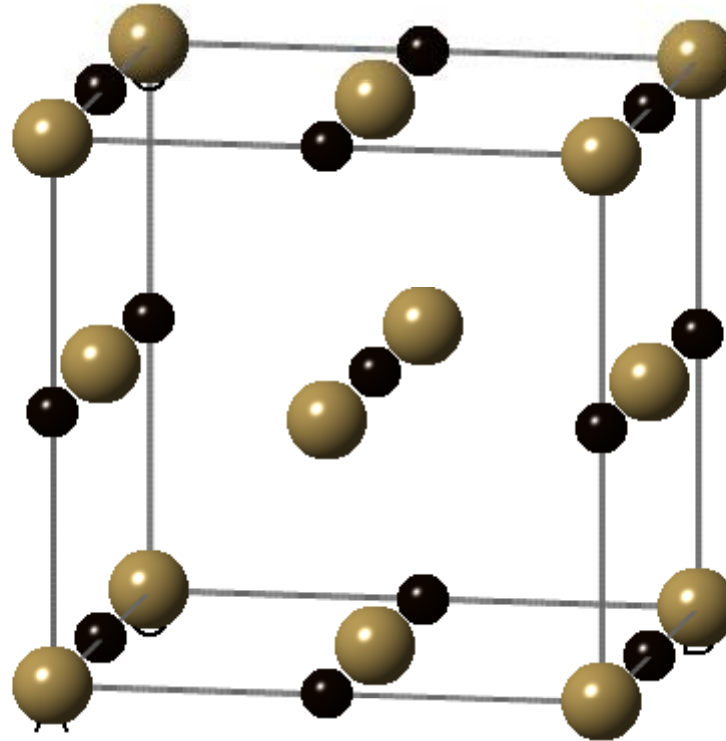
# Tantalum Carbide

## WHAT IS THE BASIS?

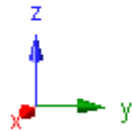


Tantalum

Carbon



$$a = b = c$$



$\left\{ \begin{array}{l} 8 \text{ atoms must be defined} \\ 4 \text{ equivalent lattice points in FCC} \\ 2 \text{ atoms on each lattice point} \end{array} \right\}$

For this crystal

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

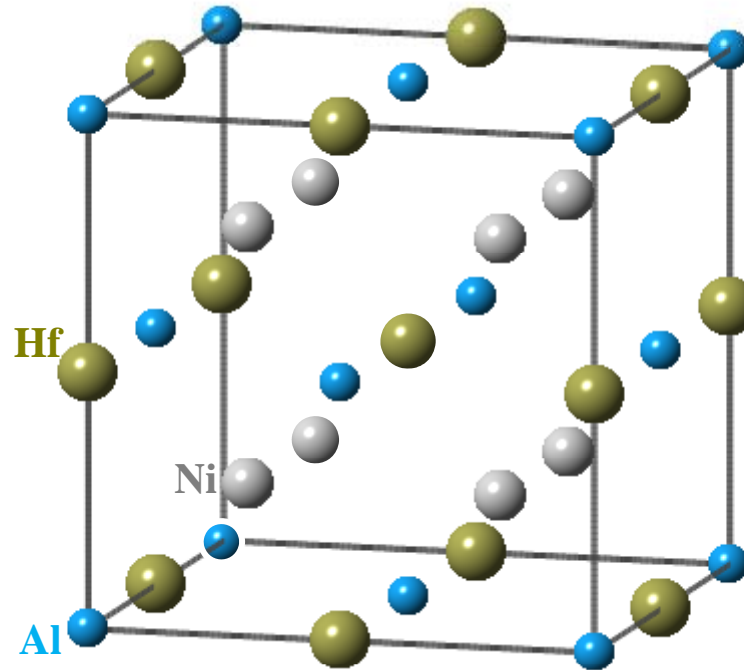
$\text{Ni}_2\text{AlHf}$   
**WHAT IS THE BASIS?**

$$a = b = c$$



Aluminum

Nickel



Hafnium

$$B =$$



**WHAT IS THE BASIS?**

$a = b = c$

Aluminum

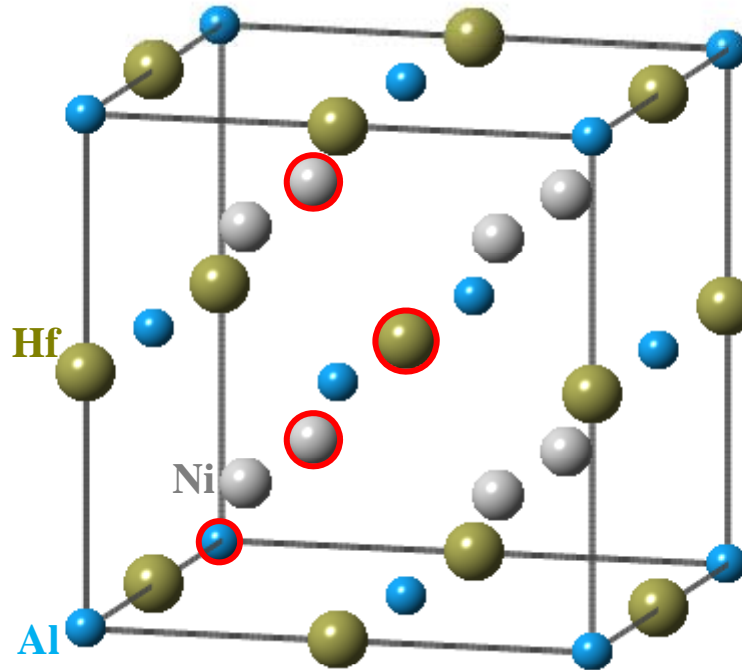
- $(0,0,0)$  ←
- $(0, \frac{1}{2}, \frac{1}{2})$
- $(\frac{1}{2}, 0, \frac{1}{2})$
- $(\frac{1}{2}, \frac{1}{2}, 0)$

Nickel

- $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$  ←
- $(\frac{3}{4}, \frac{3}{4}, \frac{3}{4})$
- $(\frac{1}{4}, \frac{3}{4}, \frac{3}{4})$
- $(\frac{3}{4}, \frac{1}{4}, \frac{3}{4})$
- $(\frac{3}{4}, \frac{3}{4}, \frac{1}{4})$
- $(\frac{3}{4}, \frac{1}{4}, \frac{1}{4})$
- $(\frac{1}{4}, \frac{3}{4}, \frac{1}{4})$
- $(\frac{1}{4}, \frac{1}{4}, \frac{3}{4})$  ←

Hafnium

- $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$  ←
- $(\frac{1}{2}, 0, 0)$
- $(0, \frac{1}{2}, 0)$
- $(0, 0, \frac{1}{2})$



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

**CsCl crystal structure**

