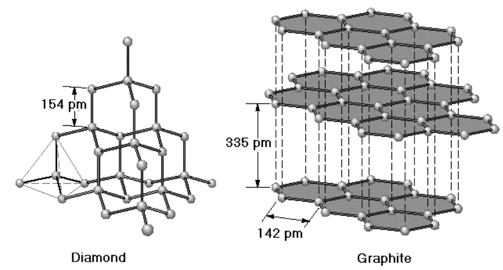
1

# Types of Solids

| TYPE | EXAMPLE | FORCE |
|---|---|---|
| Ionic | NaCl, $CaF_2$, ZnS | Ion-ion |
| Metallic | Na, Fe | Metallic |
| Molecular | Ice, $I_2$ | Dipole<br>Ind. dipole |
| Network | Diamond<br>Graphite | Extended<br>covalent |

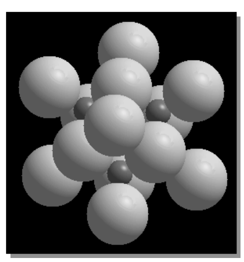
2




3

# Properties of Solids

1. Molecules, atoms or ions locked into a CRYSTAL LATTICE
2. Particles are CLOSE together
3. STRONG IM forces
4. Highly ordered, rigid, incompressible



ZnS, zinc sulfide

4

## CRYSTALLINE SOLIDS
### Crystal Lattices and Unit Cells

- **Crystal Lattice:** The ordered structure of a crystal. (or the geometric arrangement of the lattice points of a crystal).
- **Unit Cells:** The smallest "box-like" unit from which crystals can be constructed by stacking the units in three-dimensions. Each "box" has faces which are parallelograms.

5

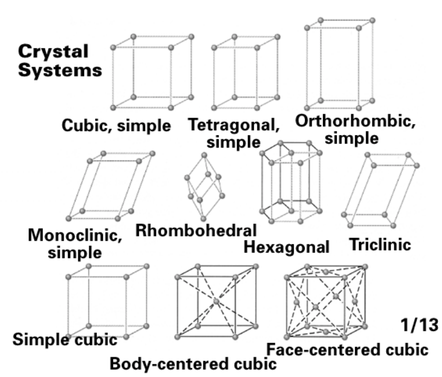
# Crystal Lattices

Regular 3-D arrangements of equivalent LATTICE POINTS in space.

The lattice points define UNIT CELLS, the smallest repeating internal unit that has the symmetry characteristic of the solid.

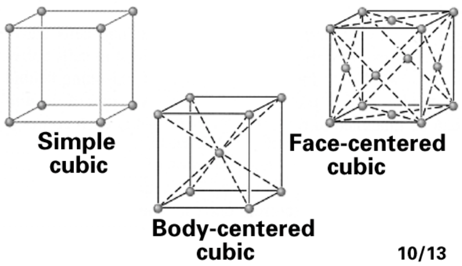
There are 7 basic crystal systems, but we are only concerned with CUBIC.

6



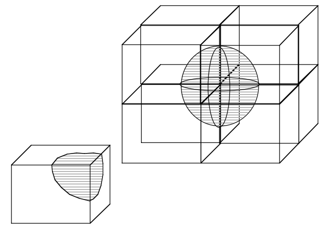
7

## Crystal Systems

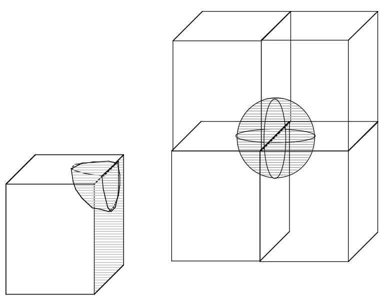



10/13

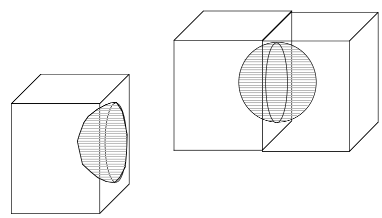
8



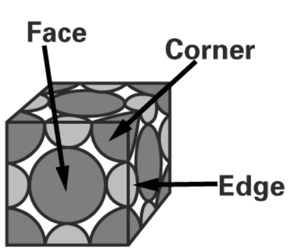
9



10



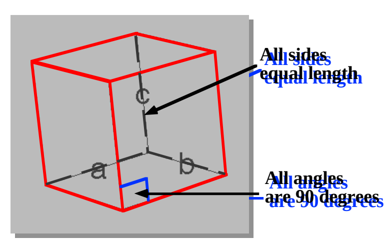
11




5/5

12

## Cubic Unit Cells



13

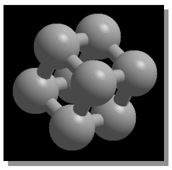
# Cubic Unit Cells

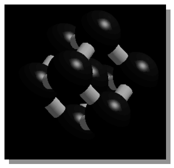
Metals have unit cells that are

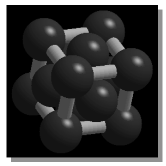
¥ simple cubic (SC)

¥ body centered cubic (BCC)

¥ face centered cubic (FCC)







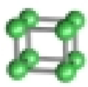
14

## Cubic Unit Cells
### Another Representation

- **Simple cubic unit cell (SC):** Lattice points are situated only at the corners of a unit cell.
- **Body-centered unit cell (BCC):** A cubic unit cell in which there is a lattice point in the center of the cell (as well as at the corners).
- **Face-centered unit cell (FCC):** A cubic unit cell in which there are lattice points in the center of each face (as well as at the corners).

15

# Simple Cubic Unit Cell

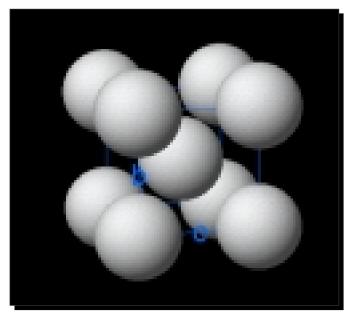


¥ Simple cubic unit cell.

¥ Note that each atom is at a corner of a unit cell and is shared among 8 unit cells.

16

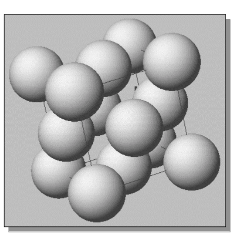
## Body-Centered Cubic Unit Cell

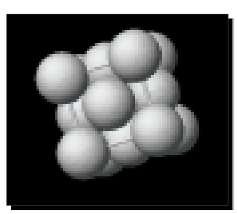


17

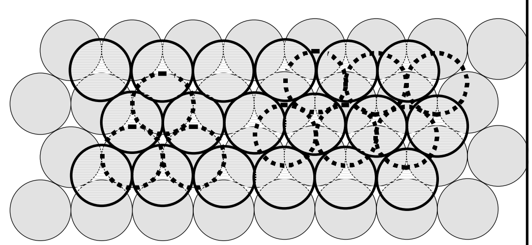
# Face Centered Cubic Unit Cell

Atom at each cube corner plus atom in each cube face.

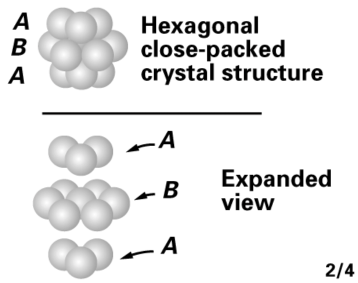




18



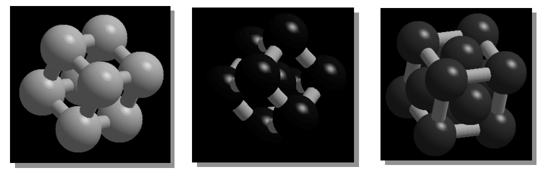
19




20

## Number of Atoms per Unit Cell

| Unit Cell Type | Net Number Atoms |
|---|---|
| FCC | 4 |
| SC | 1 |
| BCC | 2 |



21

## Finding the Lattice Type

**PROBLEM** Al has density = 2.699 g/cm$^3$ and Al radius = 143 pm. Verify that Al is FCC.

**SOLUTION**

1. Calculate the density for various cell types and select the type whose density is closest to the true value.

22

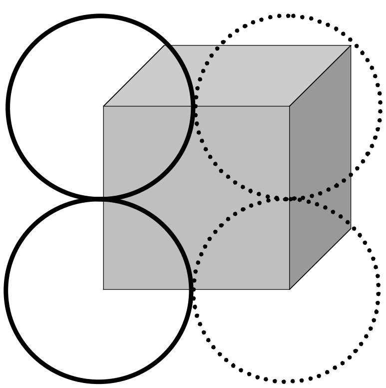
## Finding the Lattice Type

**PROBLEM** Al has density = 2.699 g/cm$^3$ and Al radius = 143 pm. Verify that Al is FCC.

**SOLUTION**

2. Use Volume , atomic weight, $N_A$ and # of atoms/cell to calculate density.

23

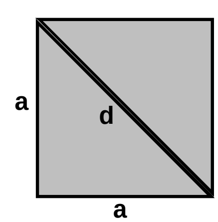


24

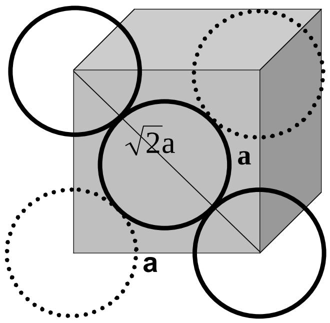
## Finding the Lattice Type

### Pythagorean theorem

- The sum of the squares of the two short sides of a right triangle equals the square of the hypotenuse.
- $a^2 + a^2 = 2a^2 = d^2$, or
- $d = a\sqrt{2}$. ,

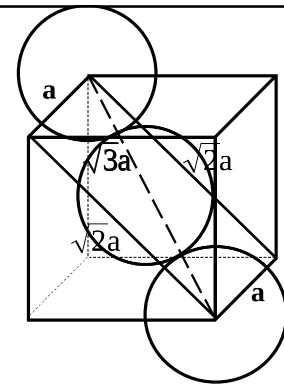


25




FCC

26




27

## Finding the Lattice Type

PROBLEM Al has density = 2.699 g/cm$^3$ and Al radius = 143 pm. Verify that Al is FCC.

**for a simple cubic** $a = 2r_{Al} = 286$ pm

**for a body centered cubic** $a = \frac{4r_{Al}}{\sqrt{3}} = 330$ pm

**for a face centered cubic** $a = \frac{4r_{Al}}{\sqrt{2}} = 404$ pm

28

**dimension in centimeters**
**1 pm = $10^{-10}$ centimeter**

**for a simple cubic** **$2.86 \times 10^{-8}$ cm**

**for a body centered cubic** **$3.30 \times 10^{-8}$ cm**

**for a face centered cubic** **$4.04 \times 10^{-8}$ cm**

29

## cell volume

**for a SC** $V = (2.86 \times 10^{-8}\ cm)^3 = 2.34 \times 10^{-23}\ cm^3$

**for a BCC** $V = (3.30 \times 10^{-8}\ cm)^3 = 3.60 \times 10^{-23}\ cm^3$

**for a FCC** $V = (4.04 \times 10^{-8}\ cm)^3 = 6.62 \times 10^{-23}\ cm^3$

30

**Atomic weight of Al = 26.9815 g/mol**

$$\frac{26.9815\ g / mol}{6.022 \times 10^{23}\ atom / mol} = 4.48 \times 10^{-23} g / atom$$

31

**if SC, the density is**

$$\frac{1\frac{\text{atom}}{\text{cell}}\times 4.48\times 10^{-23}\frac{\text{g}}{\text{atom}}}{2.34\times 10^{-23}\frac{\text{cm}^3}{\text{cell}}} = 1.92\frac{\text{g}}{\text{cm}^3} = 1.92\frac{\text{g}}{\text{ml}}$$

**if BCC, the density is**

$$\frac{2\frac{\text{atom}}{\text{cell}}\times 4.48\times 10^{-23}\frac{\text{g}}{\text{atom}}}{3.60\times 10^{-23}\frac{\text{cm}^3}{\text{cell}}} = 2.49\frac{\text{g}}{\text{cm}^3} = 2.49\frac{\text{g}}{\text{ml}}$$

32

**if FCC density is**

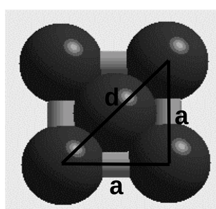
$$\frac{4\frac{\text{atom}}{\text{cell}}\times 4.48\times 10^{-23}\frac{\text{g}}{\text{atom}}}{6.61\times 10^{-23}\frac{\text{cm}^3}{\text{cell}}} = 2.71\frac{\text{g}}{\text{cm}^3} = 2.71\frac{\text{g}}{\text{ml}}$$

**The density of Al is 2.69. Since 2.69 ≈ 2.71, aluminum crystalizes in a FCC cell.**

33

# Finding the Lattice Type

**PROBLEM Al has density = 2.699 g/cm$^3$ and Al radius, $r_{Al}$ = 143 pm. Verify that Al is FCC.**




34

# Finding the Lattice Type

**For any cube the volume, V = a$^3$.**

- **In the case at hand d = 4$r_{Al}$ and**
- **4$r_{Al}$ = a√2 or a = (2√2)$r_{Al}$.**
- **V = $(2\sqrt{2})^3 r_{Al}^3$**
- 

35

# Finding the Lattice Type

**PROBLEM Al has density = 2.699 g/cm$^3$ and Al radius = 143 pm. Verify that Al is FCC.**

**SOLUTION**

**If we have a FCC unit cell then the cell diagonal = 4 ¥ radius of Al = 572 pm**

**Therefore, edge = 572 pm / ˆ2 = 404 pm**

**In centimeters, edge = 4.04 x $10^{-8}$ cm**

**So, V of unit cell = (4.04 x $10^{-8}$ cm)$^3$**

**V = 6.62 x $10^{-23}$ cm$^3$**

36

# Finding the Lattice Type

density = mass• volume

= 4•26.99/6.022 x $10^{23}$(6.62 x $10^{-23}$ cm$^3$)

=

37

# Finding the Lattice Type

PROBLEM Al has density = 2.699 $g/cm^3$ and Al radius = 143 pm. Verify that Al is FCC.

SOLUTION

3. Calculate number of Al per unit cell from mass of unit cell.

38

# Finding the Lattice Type

PROBLEM Al has density = 2.699 $g/cm^3$ and Al radius = 143 pm. Verify that Al is FCC.

SOLUTION

3. Calculate number of Al per unit cell from mass of unit cell.

$$\text{Mass 1 Al atom} = \frac{26.98 \text{ g}}{\text{mol}} \cdot \frac{1 \text{ mol}}{6.022 \times 10^{23} \text{ atoms}}$$

1 atom = $4.480 \times 10^{-23}$ g, so

39

# Finding the Lattice Type

PROBLEM Al has density = 2.699 $g/cm^3$ and Al radius = 143 pm. Verify that Al is FCC.

SOLUTION

3. Calculate number of Al per unit cell from mass of unit cell.

$$\text{Mass 1 Al atom} = \frac{26.98 \text{ g}}{\text{mol}} \cdot \frac{1 \text{ mol}}{6.022 \times 10^{23} \text{ atoms}}$$

1 atom = $4.480 \times 10^{-23}$ g, so

$$\frac{1.79 \times 10^{-22} \text{ g}}{\text{unit cell}} \cdot \frac{1 \text{ atom}}{4.480 \times 10^{-23} \text{ g}} = 3.99 \text{ Al atoms/unit cell}$$

40

# Number of Atoms per Unit Cell

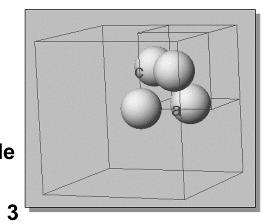
How can there be 4 atoms in a unit cell?

1. Each corner Al is 1/8 inside the unit cell.

   8 corners (1/8 Al per corner) = 1 net Al

2. Each face Al is 1/2 inside the cell

   6 faces (1/2 per face) = 3 net Al s




41

# Simple Ionic Compounds

Lattices of many simple ionic solids are built by taking a SC or FCC lattice of ions of one type and placing ions of opposite charge in the holes in the lattice.

EXAMPLE: CsCl has a SC lattice of $Cs^+$ ions with $Cl^-$ in the center.

42

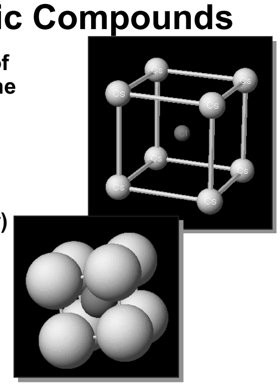
# Simple Ionic Compounds

CsCl has a SC lattice of $Cs^+$ ions with $Cl^-$ in the center.

1 unit cell has 1 $Cl^-$ ion plus

(8 corners)(1/8 $Cs^+$ per corner)

= 1 net $Cs^+$ ion.



43

# Simple Ionic Compounds

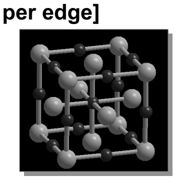
Many common salts have FCC arrangements of anions with cations in OCTAHEDRAL HOLES e.g. , salts such as CA = NaCl

¥ FCC lattice of anions ----> 4 $A^-$/unit cell

¥ $C^+$ in octahedral holes ---> 1 $C^+$ at center

+ [12 edges ¥ 1/4 $C^+$ per edge]

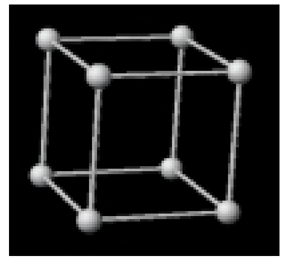
= 4 $C^+$ per unit cell



44

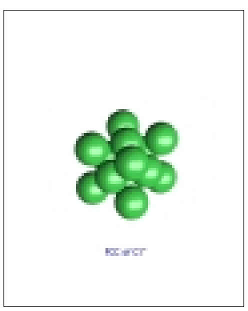
# Construction of NaCl

We begin with a cube of $Cl^-$ ions. Add more $Cl^-$ ions in the cube faces, and then add $Na^+$ ion in the octahedral holes.



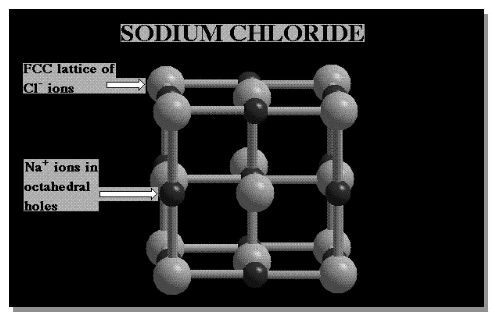
45

## The Sodium Chloride Lattice



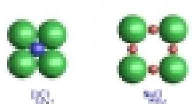
$Na^+$ ions are in OCTAHEDRAL holes in a face-centered cubic lattice of $Cl^-$ ions.

46




47

# Comparing NaCl and CsCl

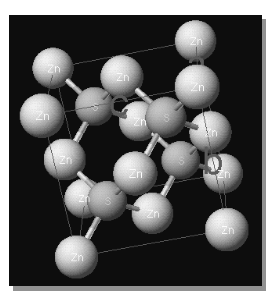


¥ Even though their formulas have one cation and one anion, the lattices of CsCl and NaCl are different.

¥ The different lattices arise from the fact that a $Cs^+$ ion is much larger than a $Na^+$ ion.

48

# Common Ionic Solids



¥ Zinc sulfide, ZnS

¥ The $S^{2-}$ ions are in TETRAHEDRAL holes in the $Zn^{2+}$ FCC lattice.

¥ This gives 4 net $Zn^{2+}$ ions and 4 net $S^{2-}$ ions.