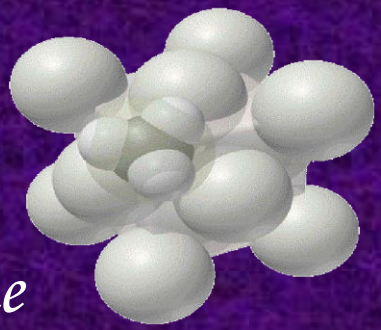
Solid State



Gases: no definite shape and volume

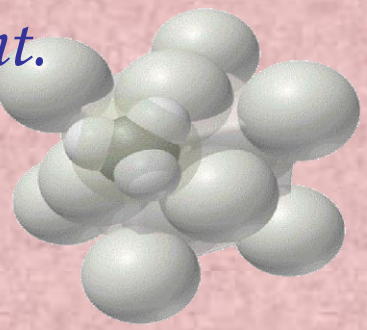
Liquids: no definite shape but definite volume

Solids: definite shape and volume

Solids: definite shape, volume and order.

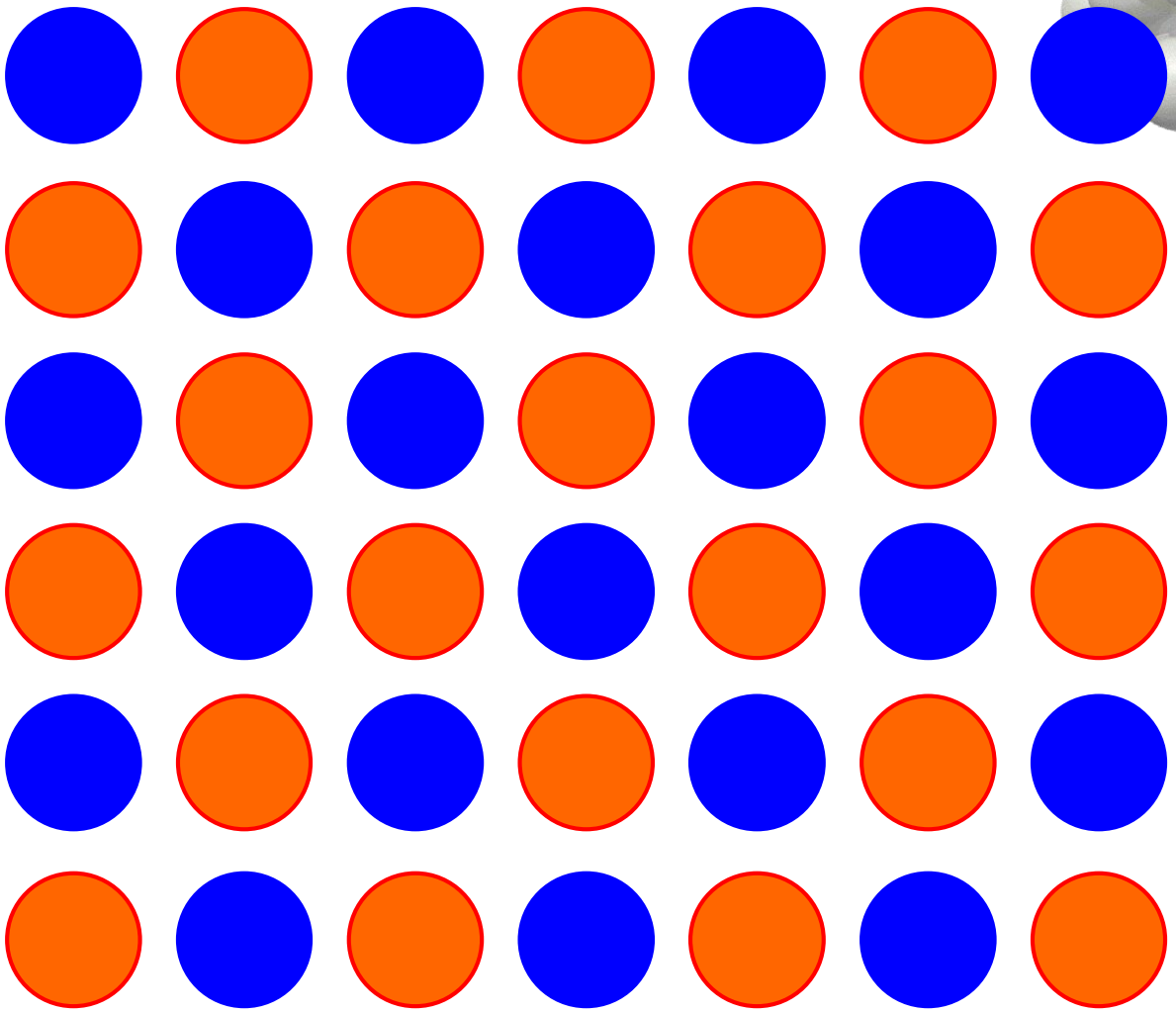
Order: definite pattern of arrangement of atoms or molecules or ions.

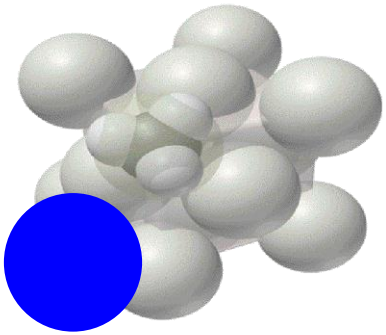
Intensive properties: do not depend on the amount.



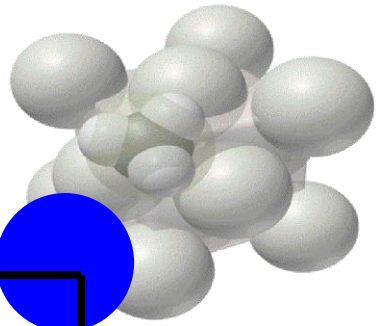
Unit Cells

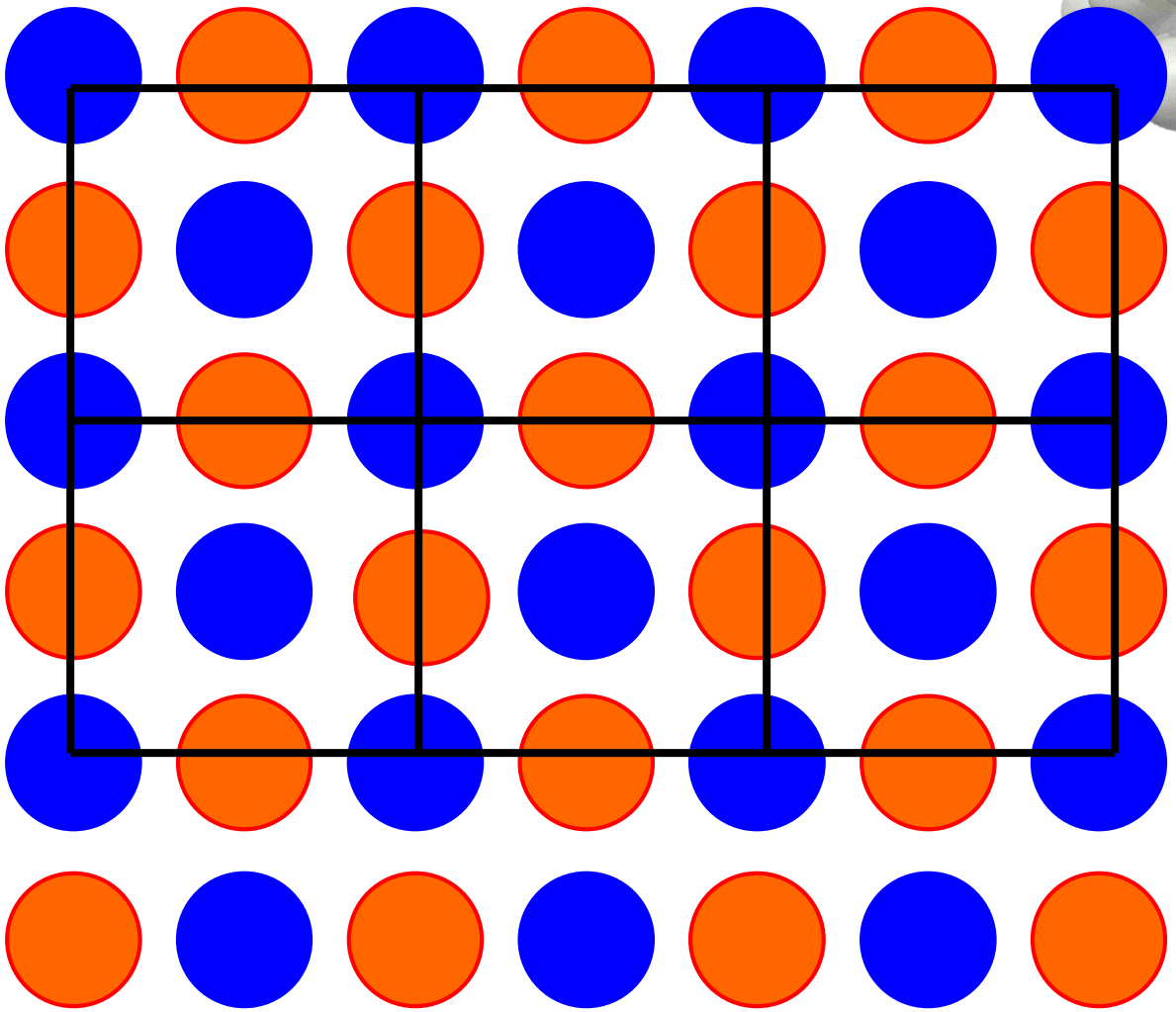
- *Smallest Repeating Unit*
- *Unit Cells must link-up – cannot have gaps between them*
- *All unit cells must be identical*



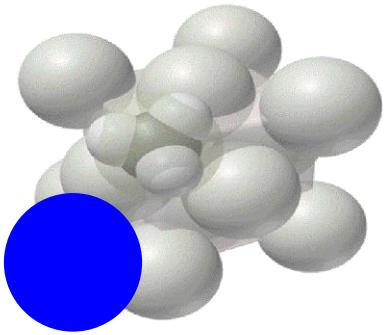


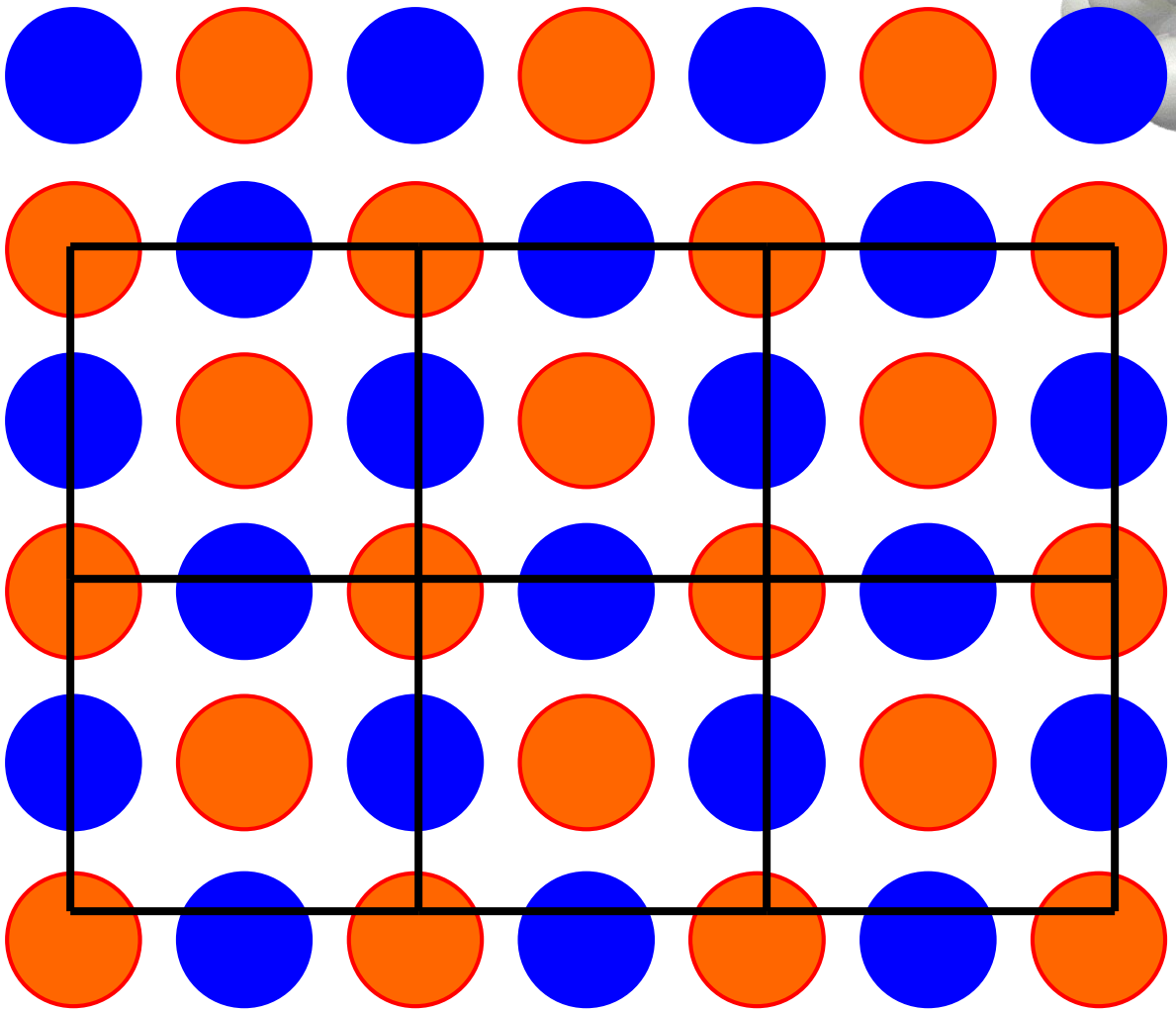
Choice of the origin is arbitrary



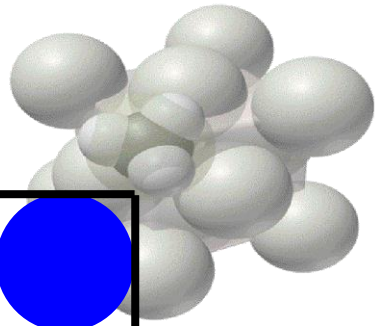


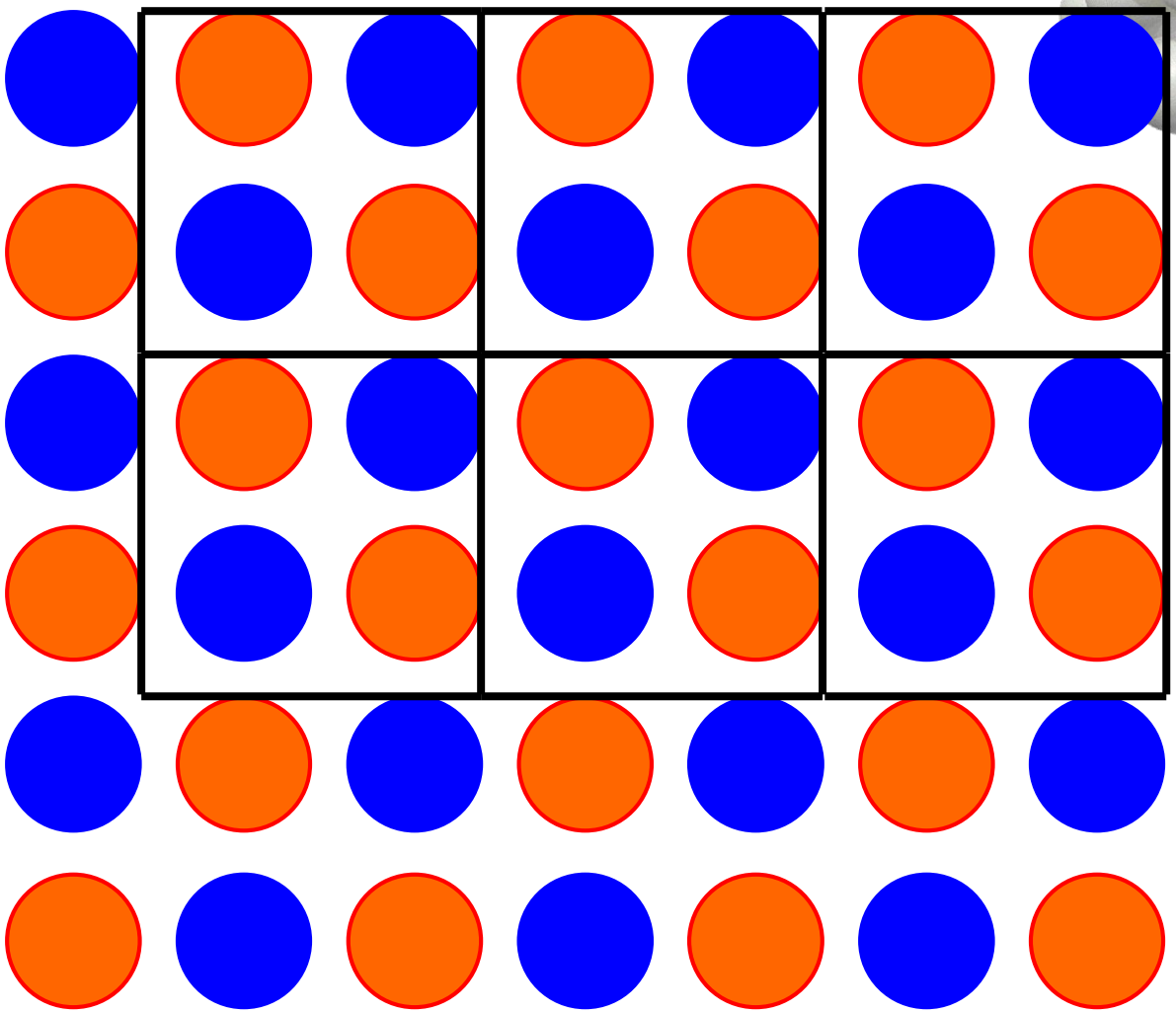
Blue atom or orange atom or



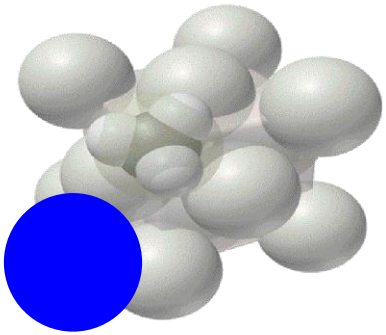


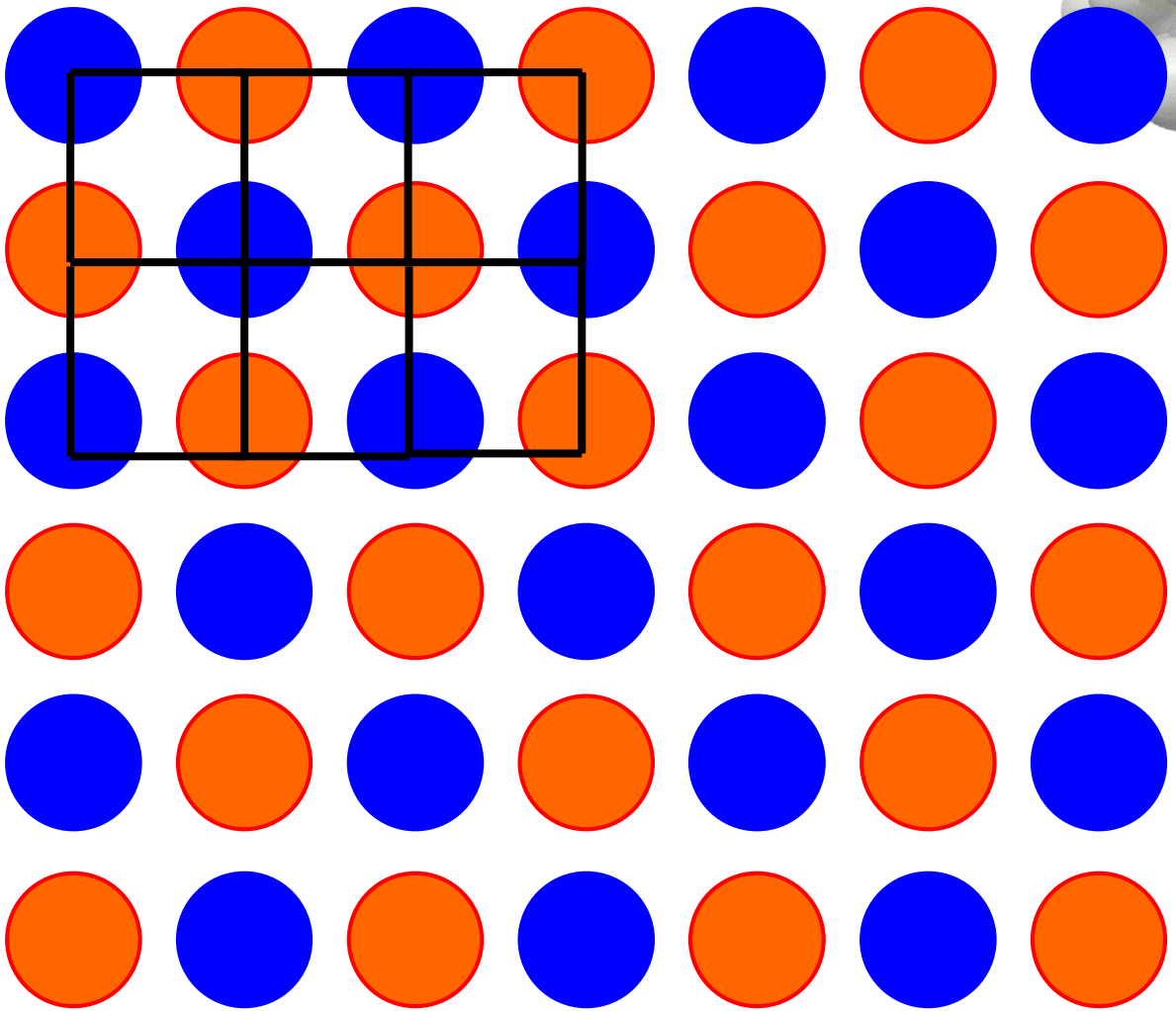
even a space!





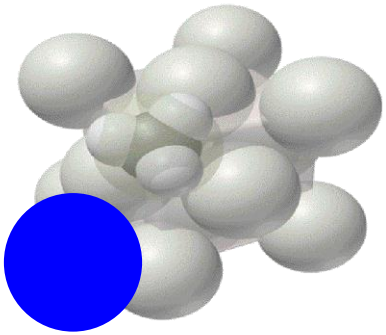
This cannot be a unit cell

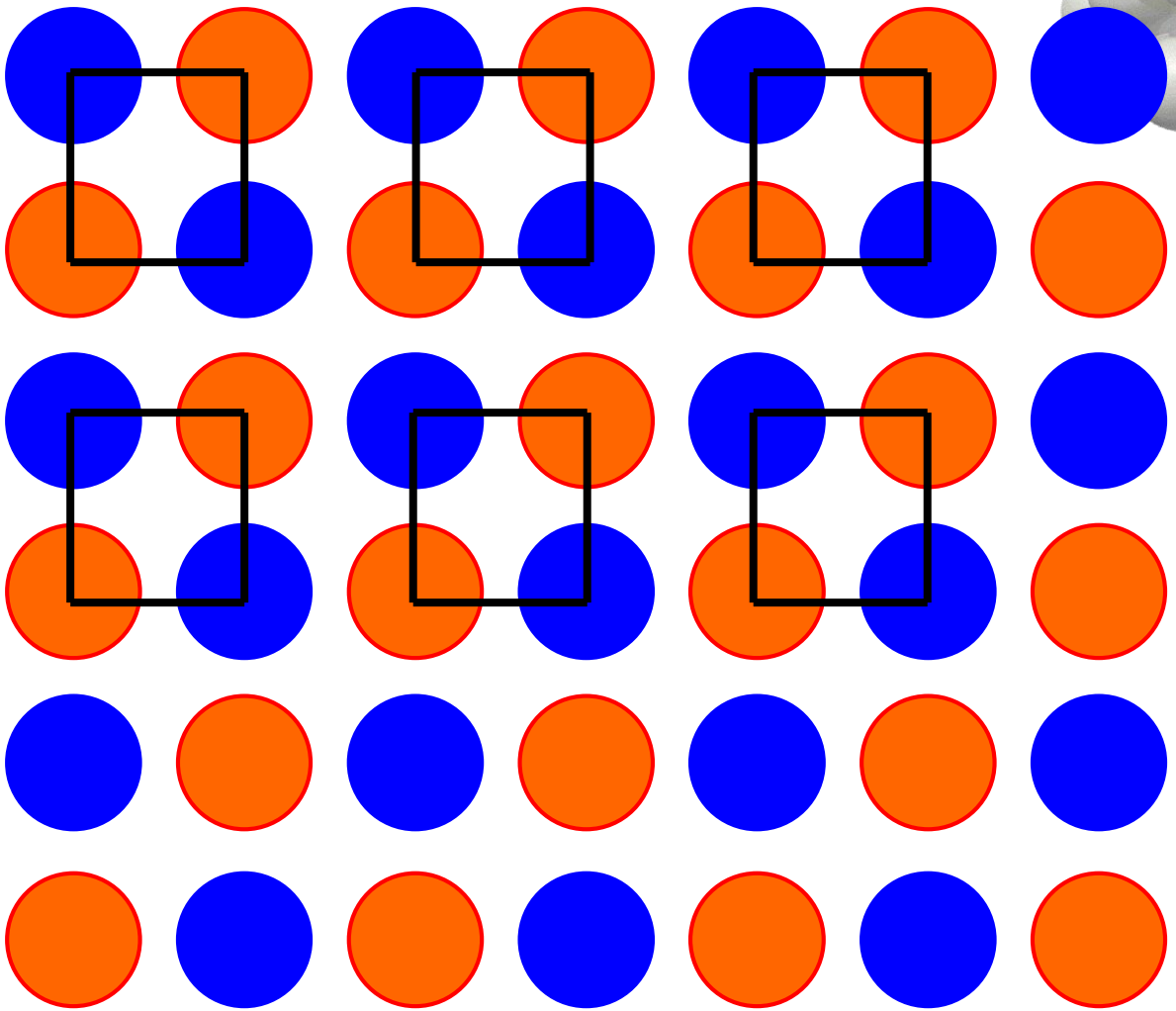




Unit cells are not identical

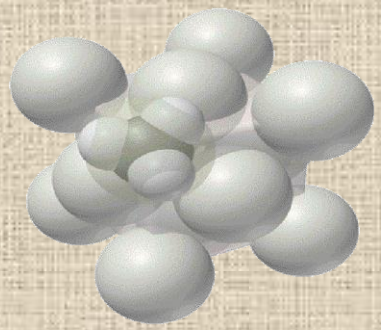
This also cannot be a unit cell





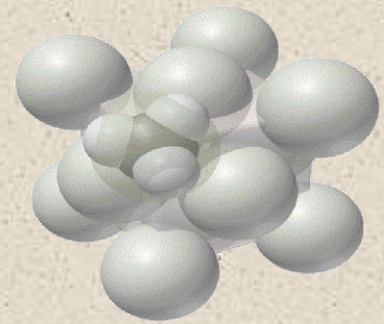
Space between unit cells not allowed

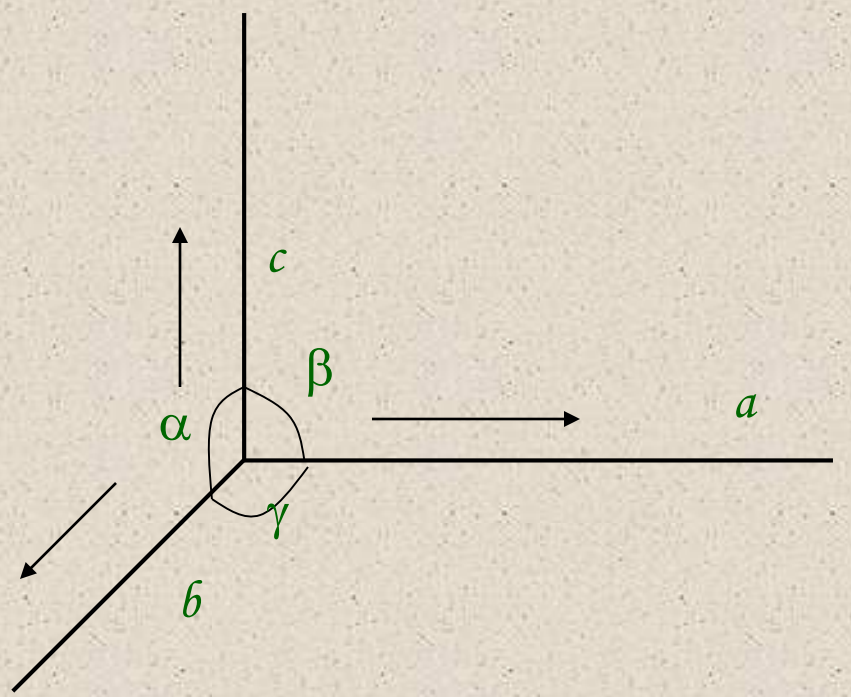
Unit cells exist in only seven shapes



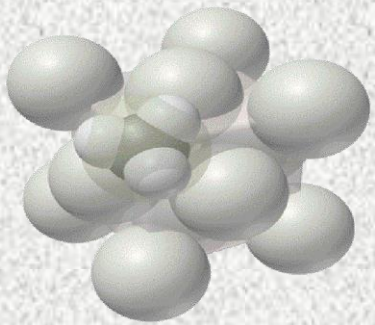
- *Cubic*
- *Orthorhombic*
- *Rhombohedral*
- *Tetragonal*
- *Triclinic*
- *Hexagonal*
- *Monoclinic*

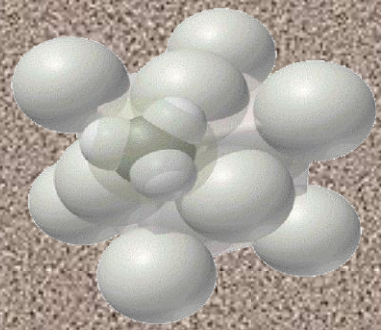
Crystal intercepts & Angles





Crystal Systems	Lattice Parameters	
	Crystal Intercepts	Crystal Angles
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^o$
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^o$
Rhombohedral	$a = b = c$	$\alpha = \beta = \gamma \neq 90^o$
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^o$
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^o$
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90^o$, $\gamma = 120^o$
Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90^o$, $\beta \neq 90^o$

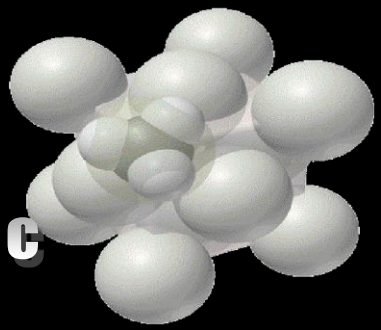




There are not more than 4 ways of arranging spheres in any shape of unit cell

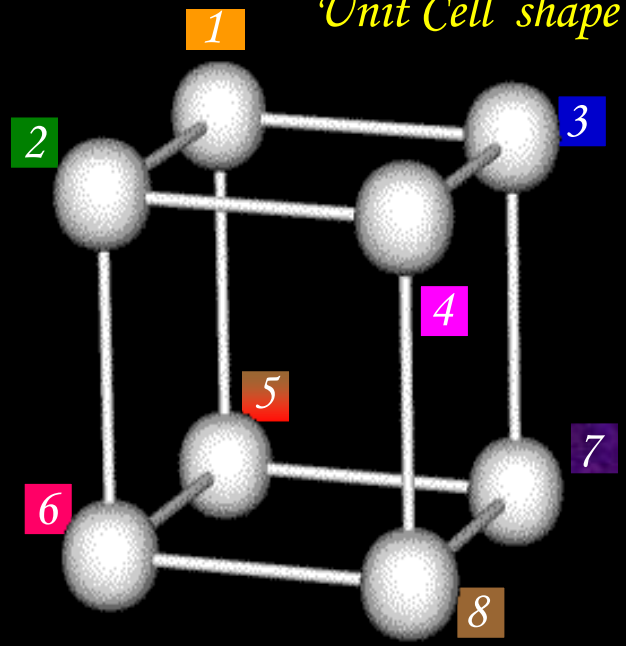
These are Primitive, Body Centered, Face Centered & End Centered

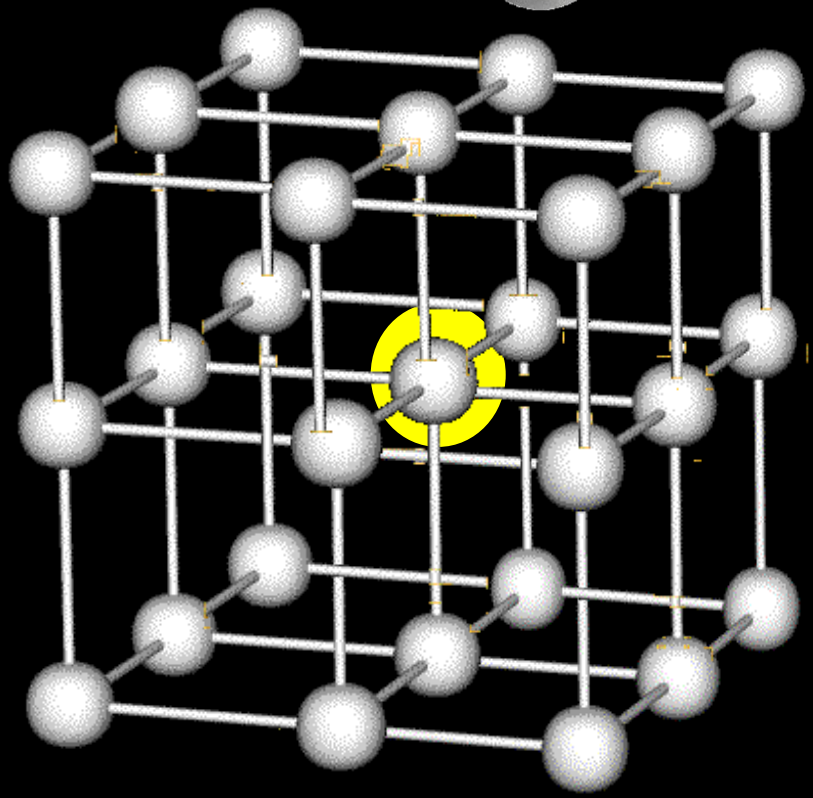
Primitive Cubic

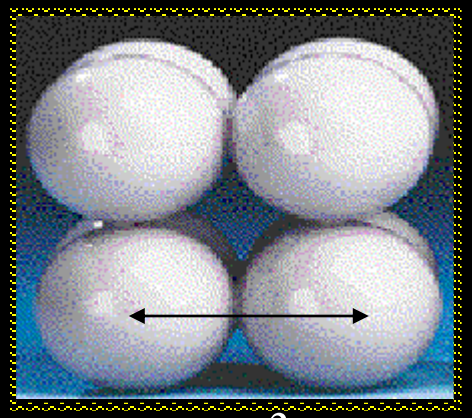


Unit Cell shape view

Simple Cubic

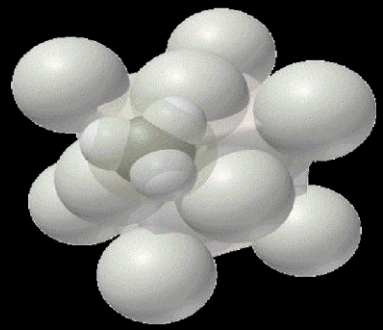




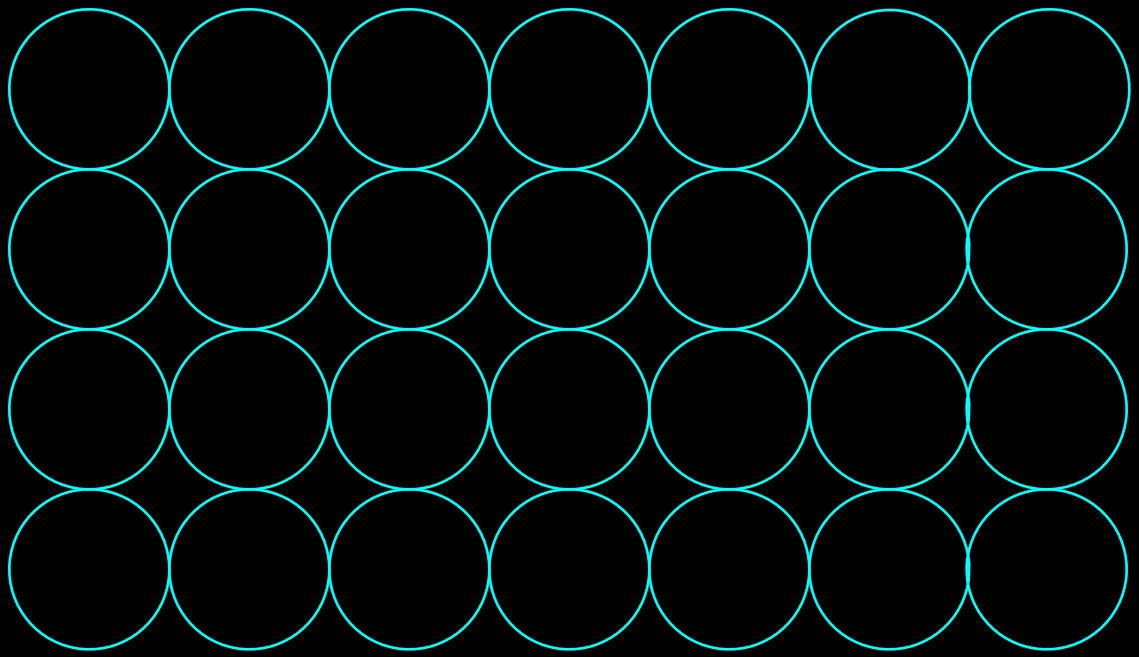


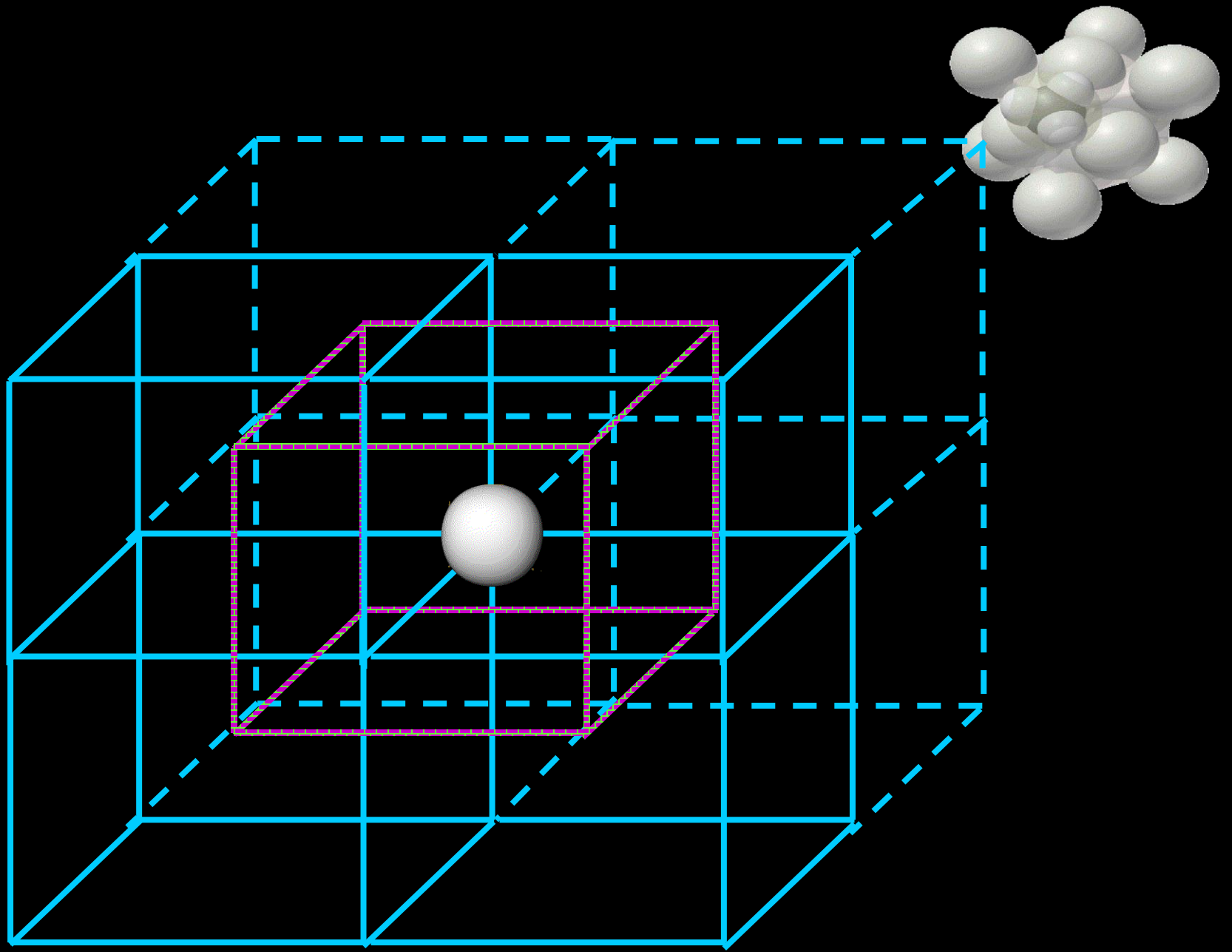
a = 2r

Unit Cell arrangement view

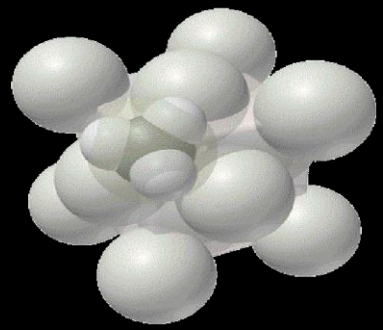


Layer arrangement view



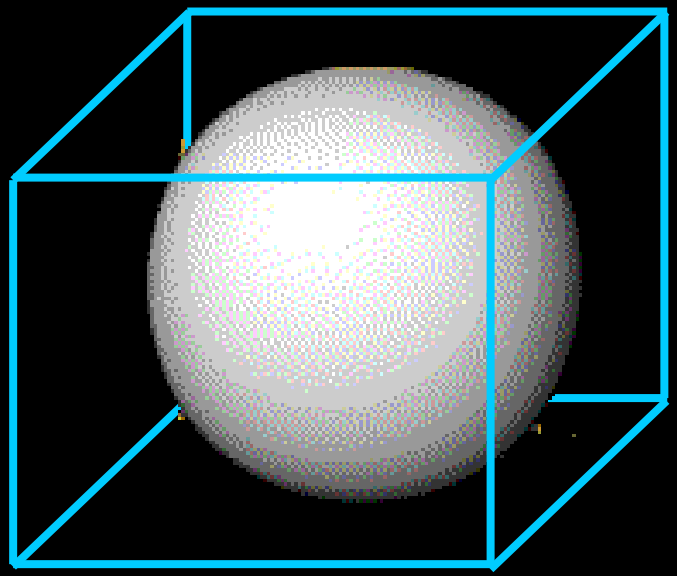


Primitive Cubic



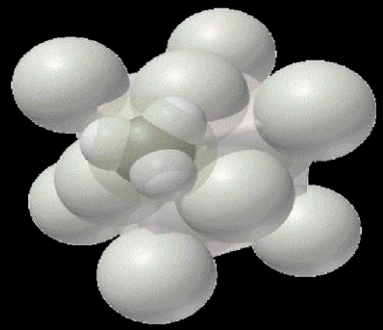
Volume occupied by a sphere in the unit cell $= \frac{1}{8} V$

Total volume occupied by all the spheres in the unit cell $= \frac{1}{8} V \times 8 = 1V$



Primitive Cubic

Packing Fraction



Fraction of the Unit cell's volume occupied by the spheres

$$= \frac{\text{Volume occupied by the spheres inside the unit cell}}{\text{volume of unit cell}}$$

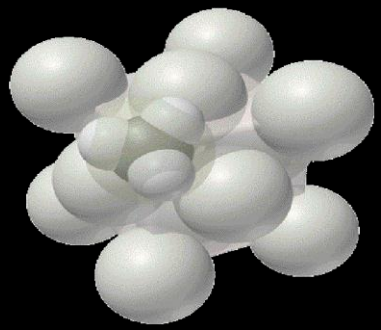
$$= \frac{\frac{4}{3}\pi r^3}{a^3}$$

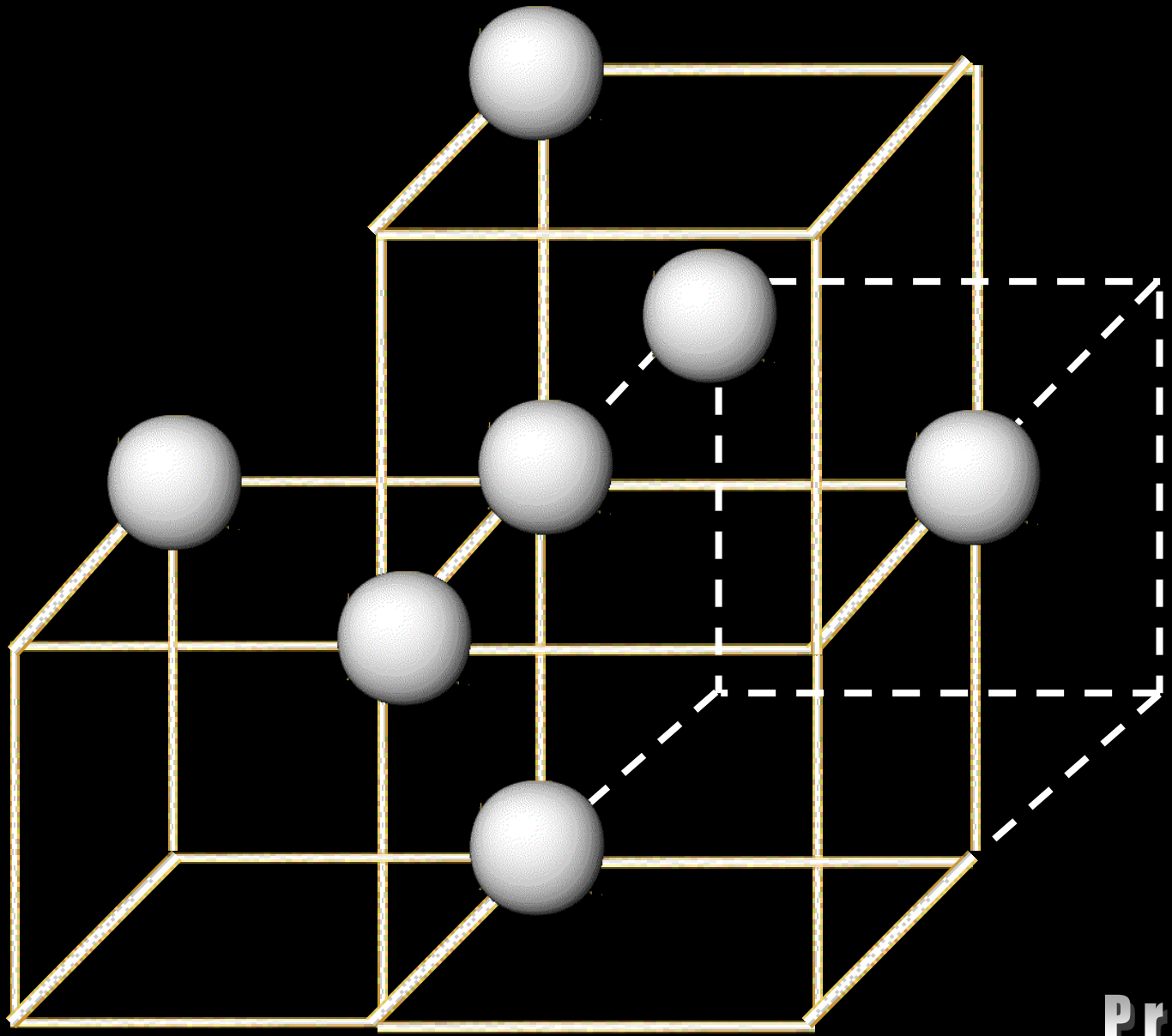
$$= \frac{\frac{4}{3}\pi r^3}{(2r)^3}$$

$$= 0.52$$

Primitive Cubic

Coordination number

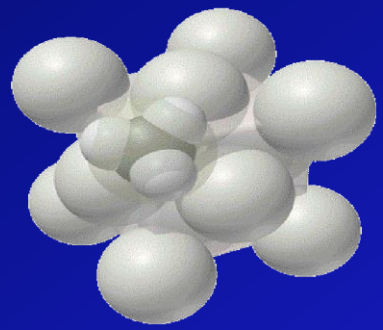




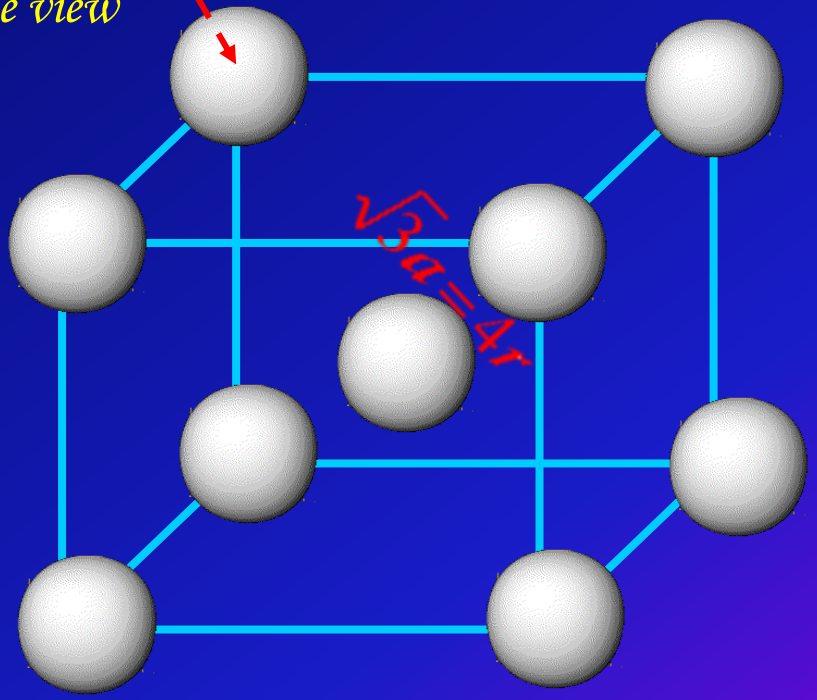
6

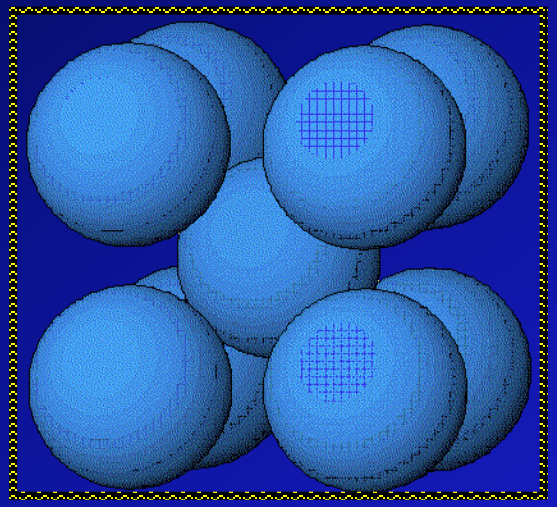
Primitive Cubic

Body Centered Cubic



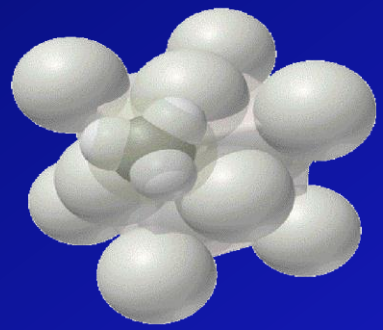
Unit Cell shape view

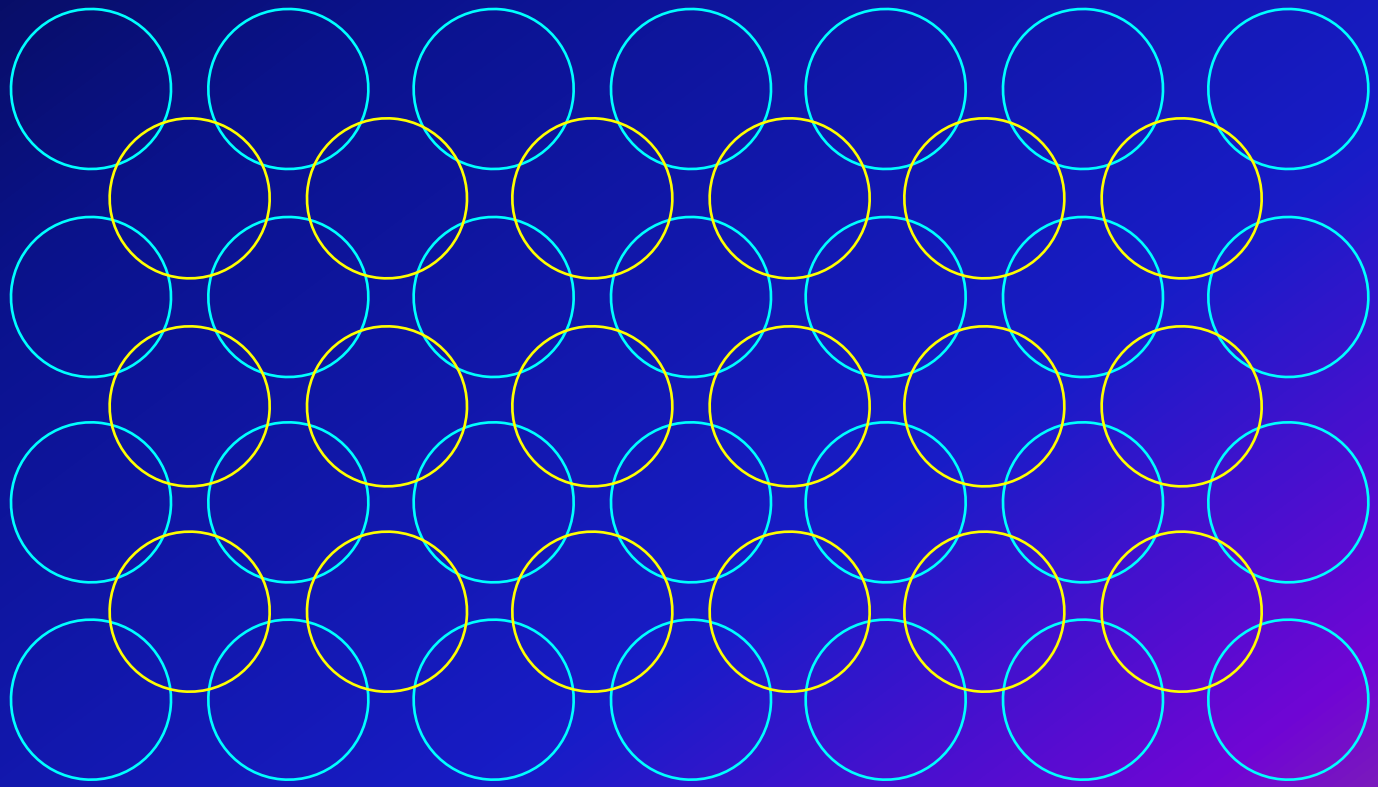


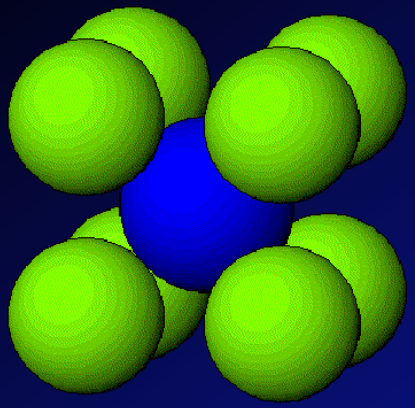


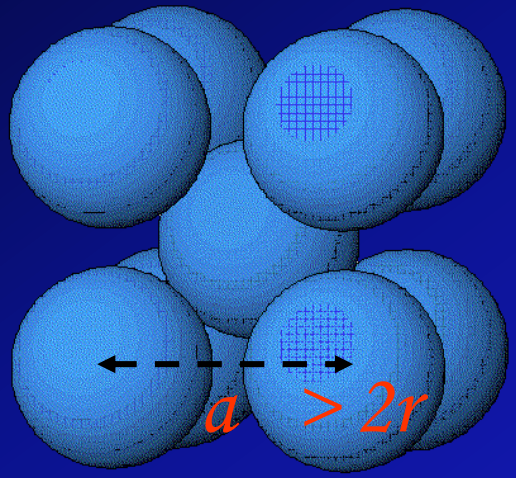
Unit Cell arrangement view

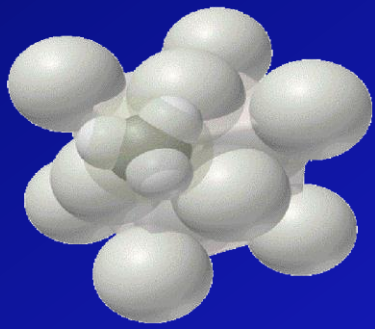
Layer arrangement view

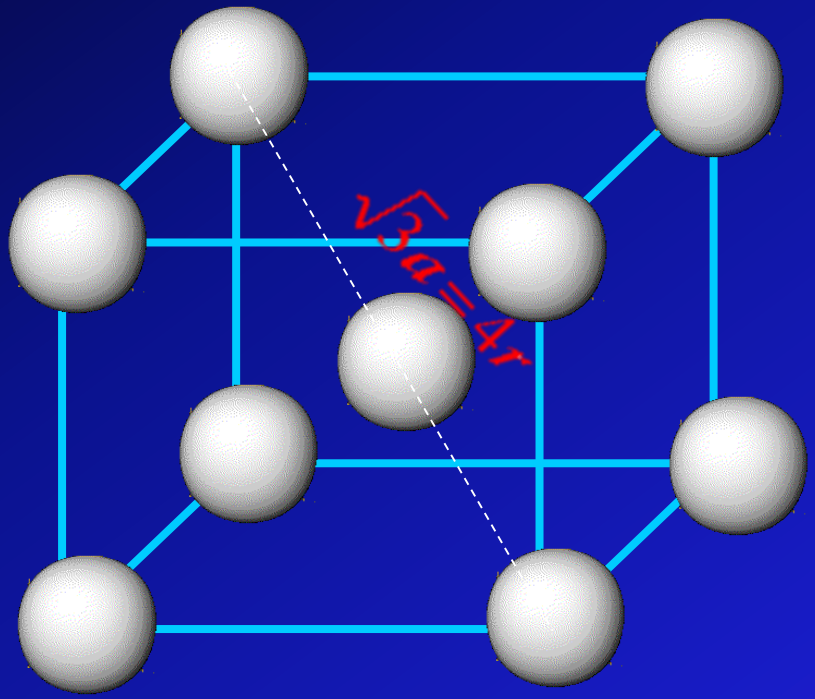








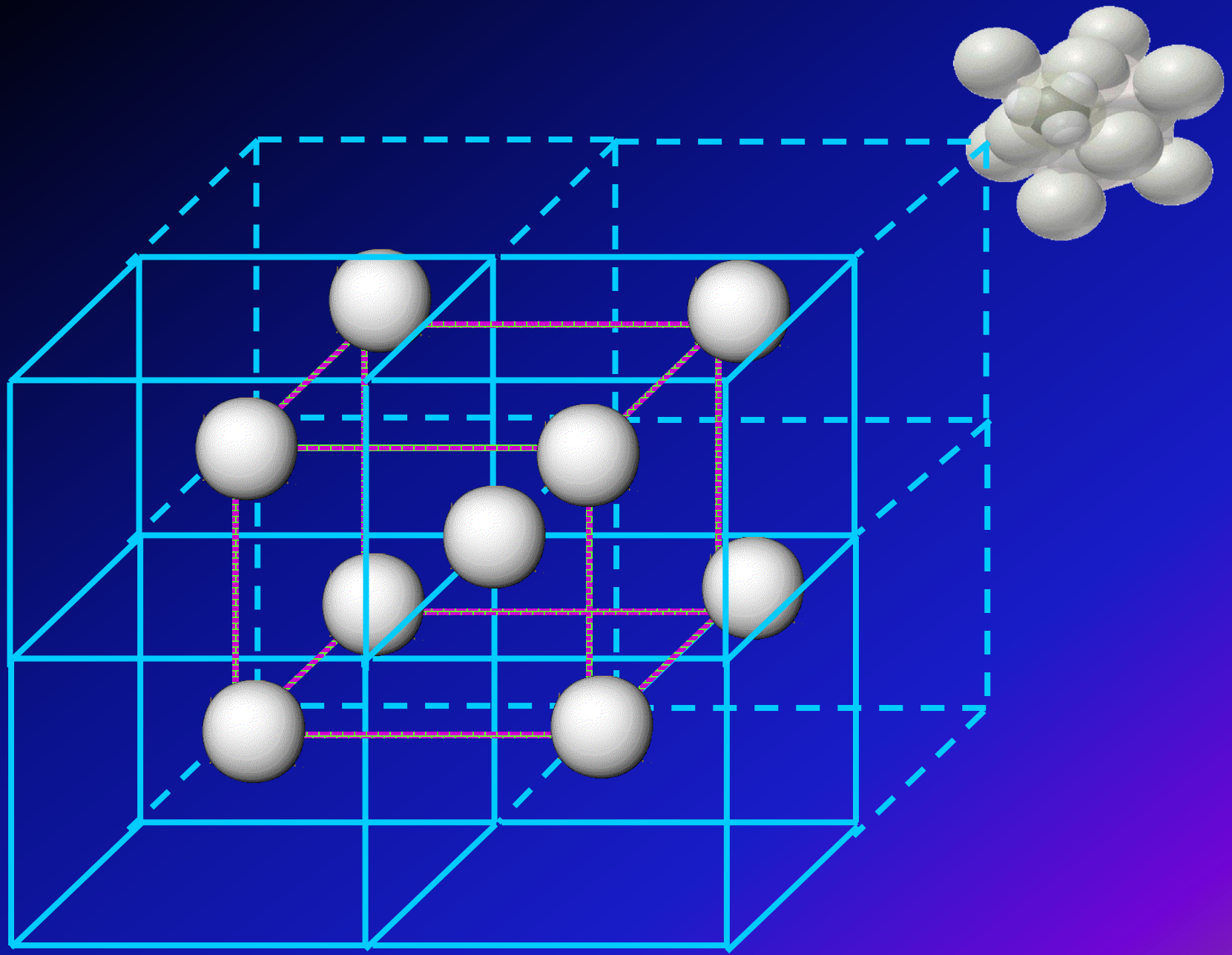




$$4r = \sqrt{3}a$$

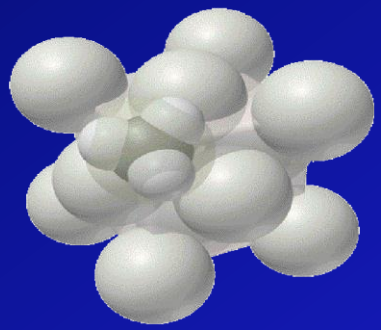
$$2r = \frac{\sqrt{3}a}{2} < a$$

Body Centered Cubic



Body Centered Cubic

Packing Fraction



Volume occupied by a corner sphere in the unit cell $= \frac{1}{8}V$

Volume occupied by the central sphere in the unit cell $= 1V$

Total Volume occupied by the spheres in the unit cell $= 2V$

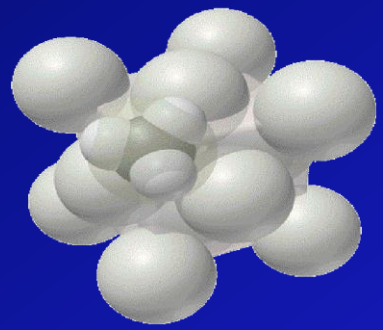
Packing Fraction

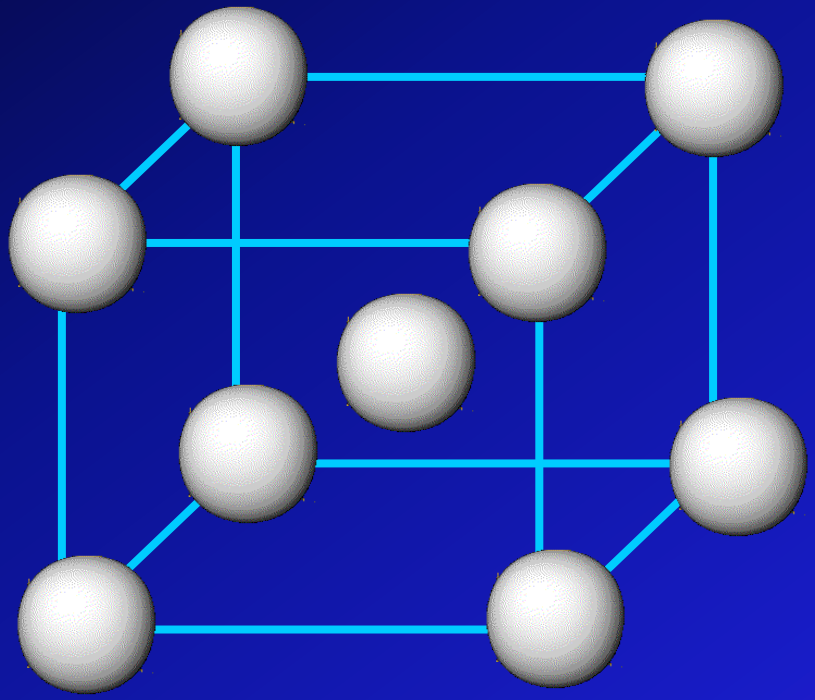
$$= \frac{2 \times \frac{4}{3}\pi r^3}{\left(\frac{4r}{\sqrt{3}}\right)^3}$$

$$= 0.68$$

Body Centered Cubic

Coordination number

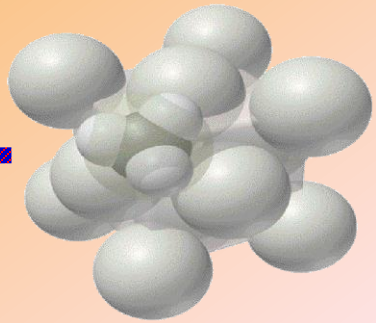




8

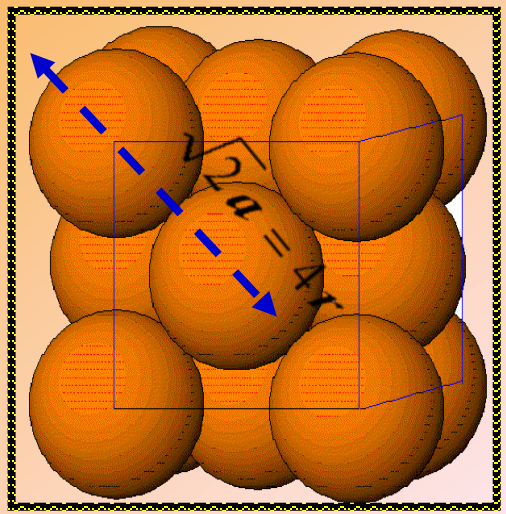
Body Centered Cubic

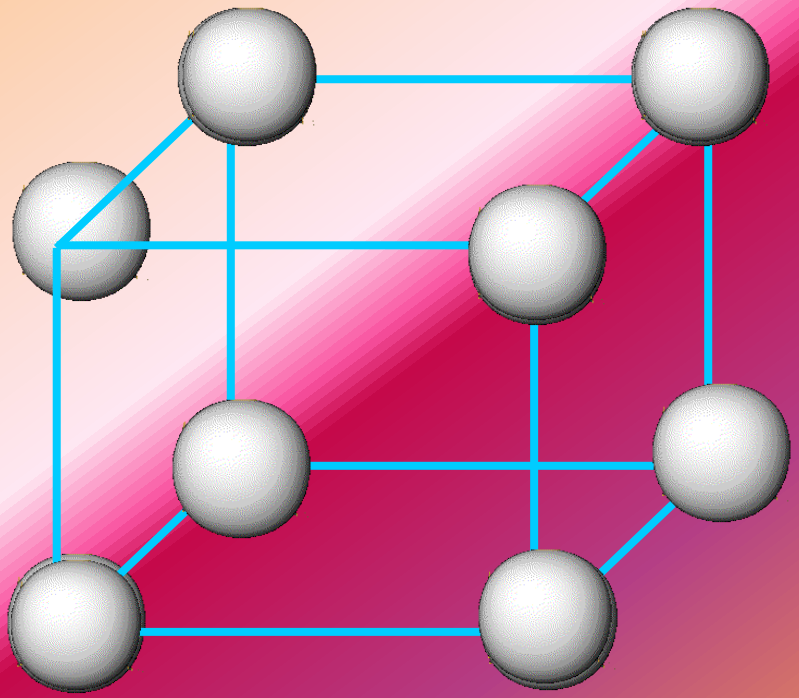
Face Centered Cubic

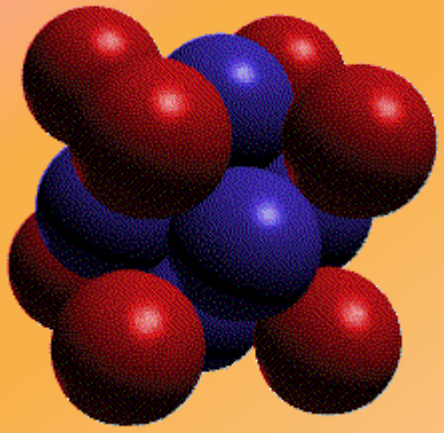


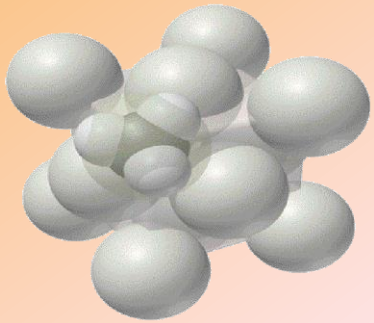
Unit Cell shape view

Unit Cell arrangement view



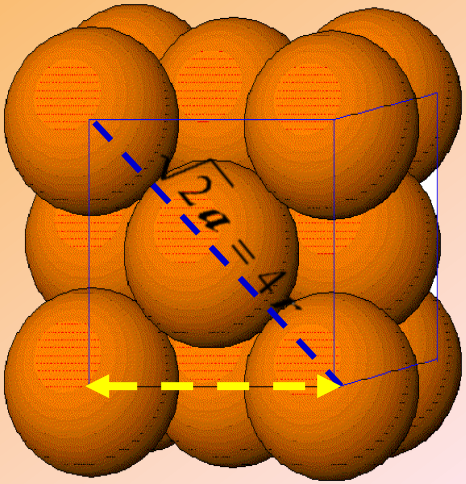






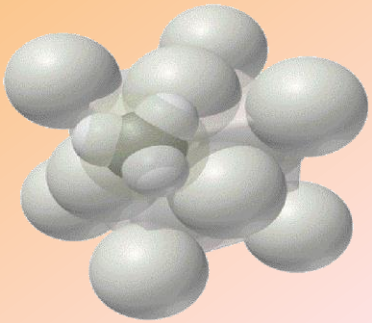
$$4r = \sqrt{2}a$$

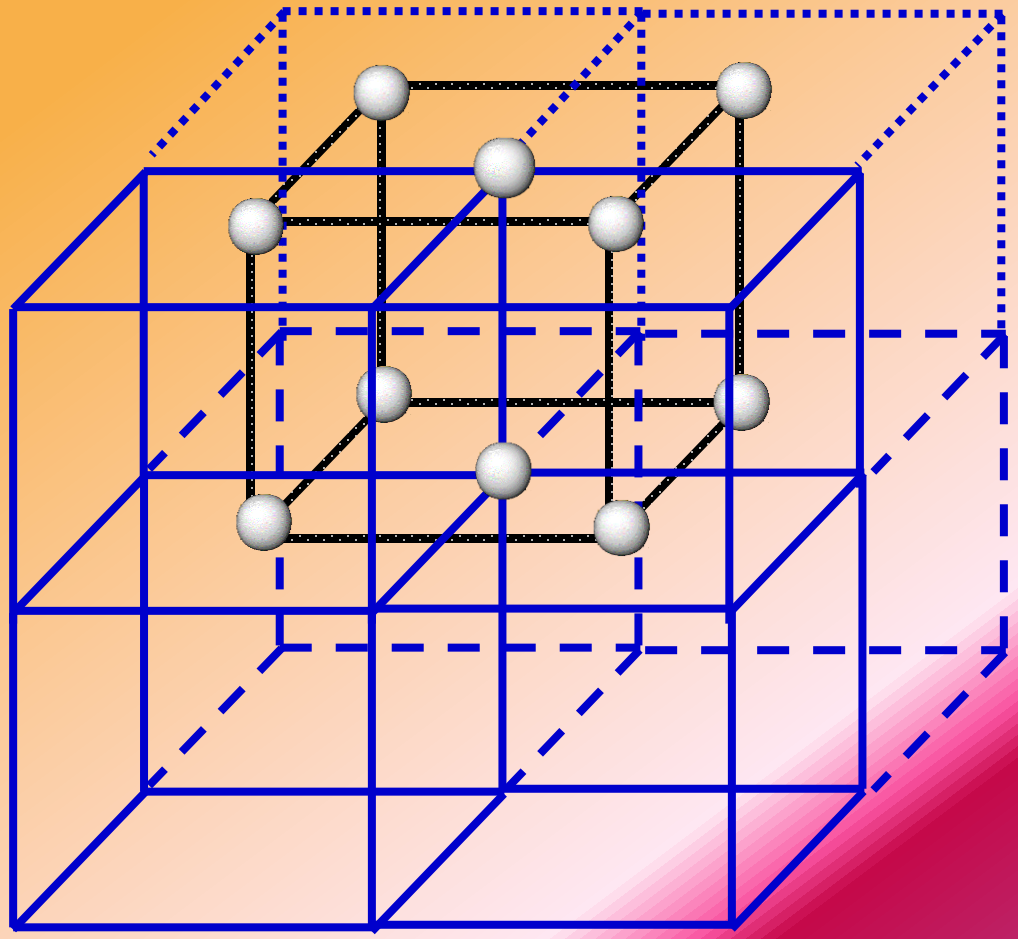
$$2r = \frac{a}{\sqrt{2}} < a$$



$a > 2r$

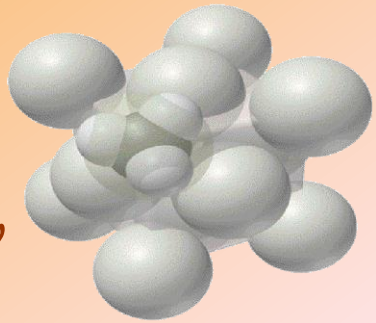
Face Centered Cubic





Face Centered Cubic

Packing Fraction



Volume occupied by a corner sphere in the unit cell $= \frac{1}{8}V$

Volume occupied by a face centered sphere in the unit cell $= \frac{1}{2}V$

Total Volume occupied by the spheres in the unit cell

$$= 8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 4$$

Packing Fraction

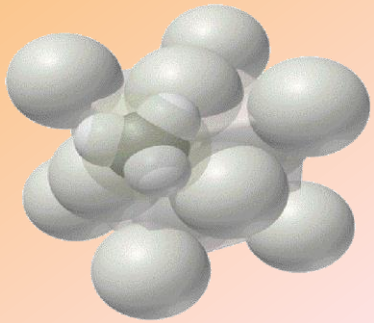
$$= \frac{4 \times \frac{4}{3}\pi r^3}{\left(\frac{4r}{\sqrt{2}}\right)^3}$$

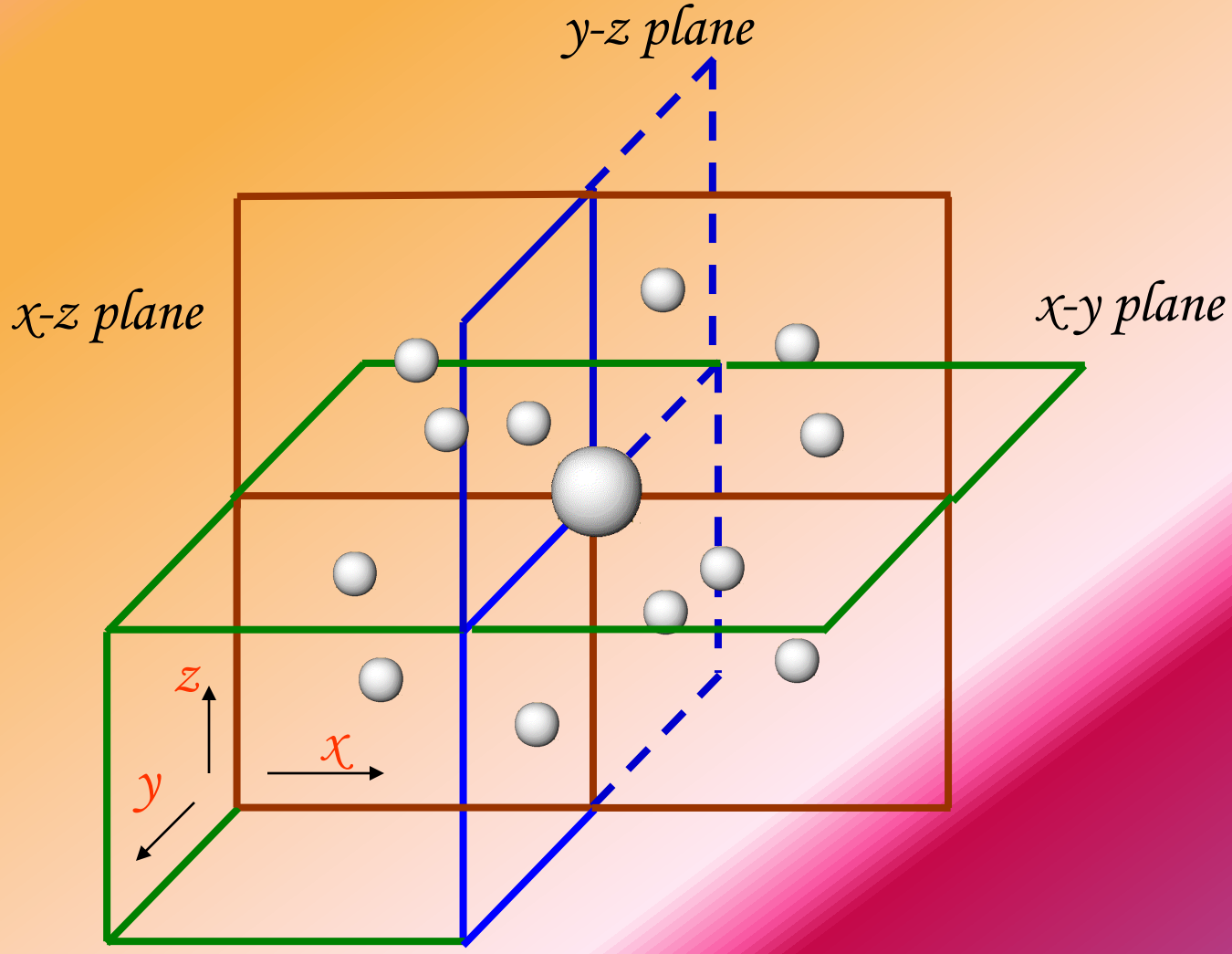
$$= 0.74$$

Highest Packing Fraction of all shapes and of all arrangements

Face Centered Cubic

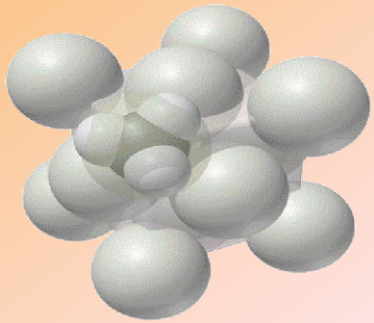
Coordination number

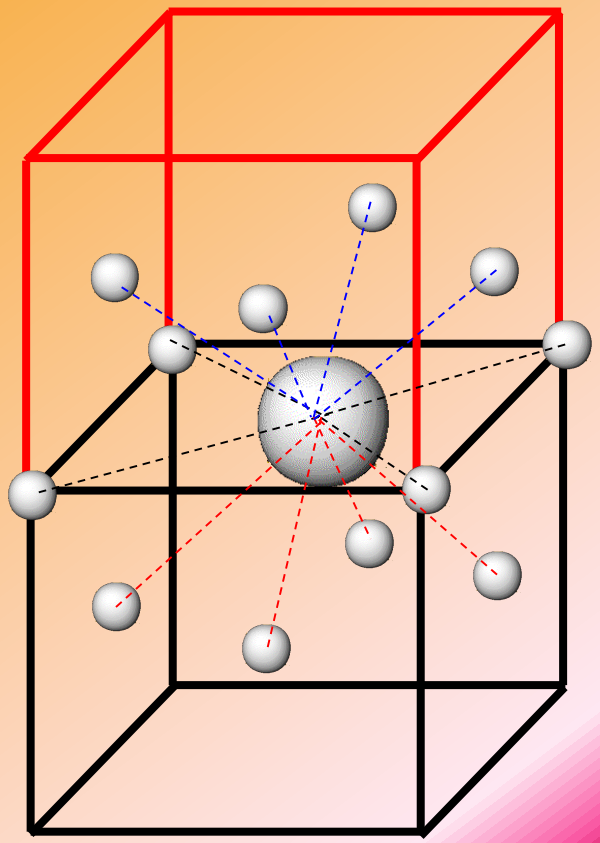


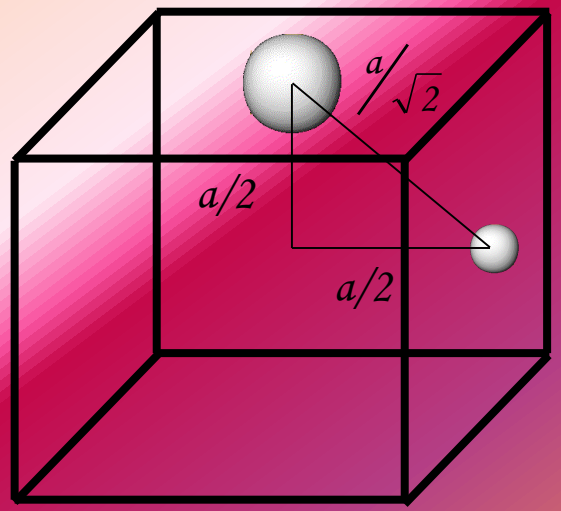


Face Centered Cubic

Coordination number

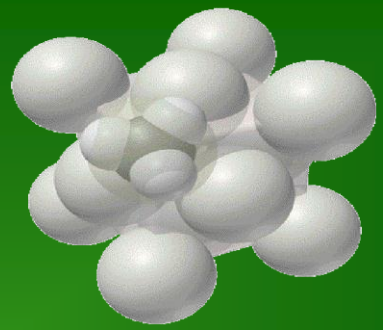


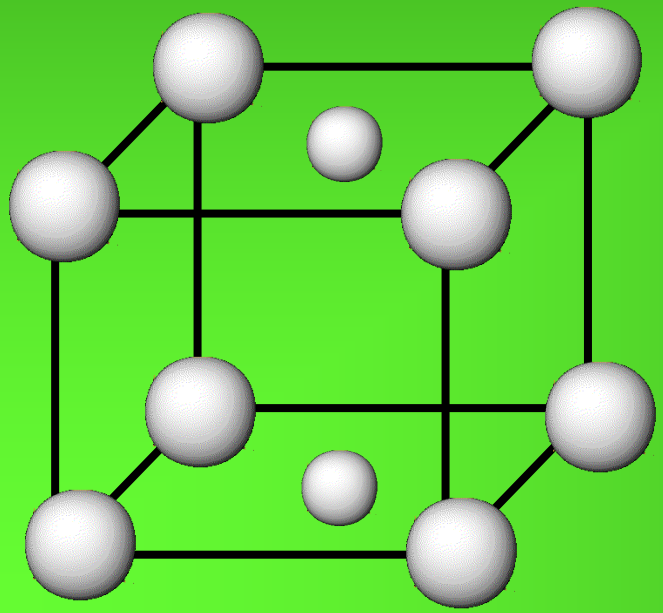


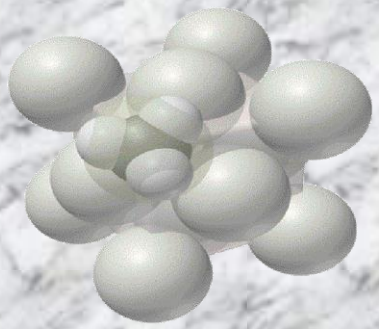


Face Centered Cubic

End Centered



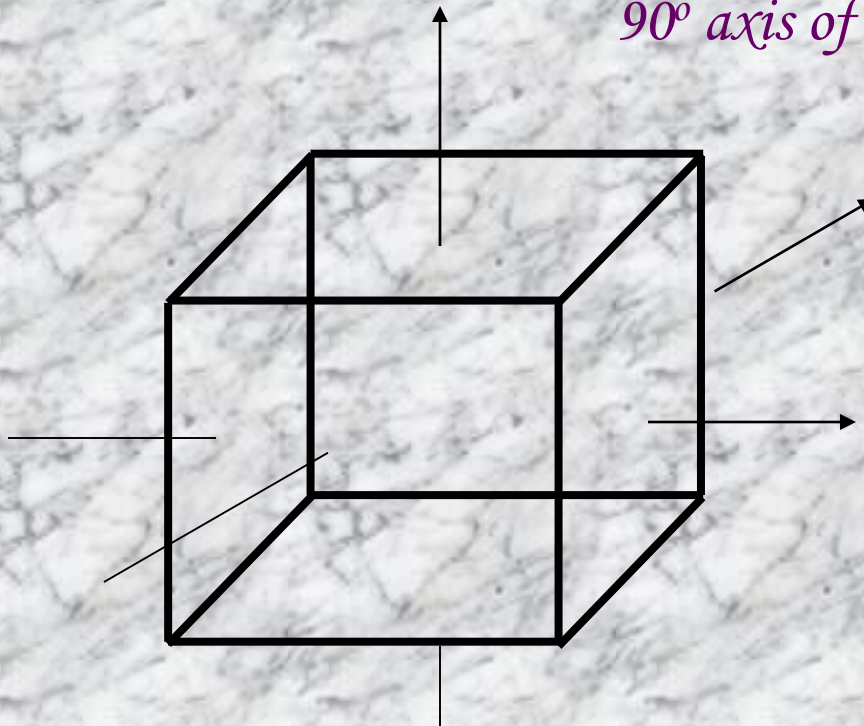


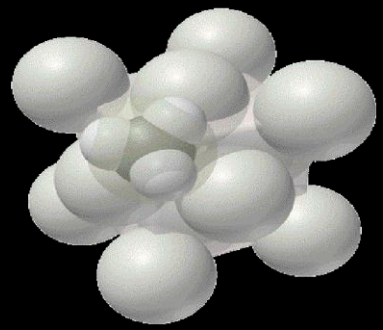


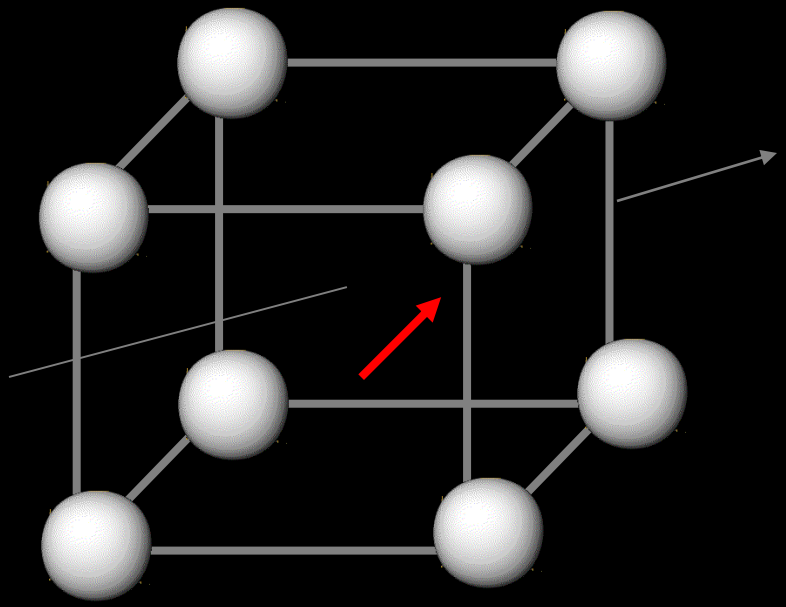
Out of all the twenty eight possible unit cells only 14 exist !

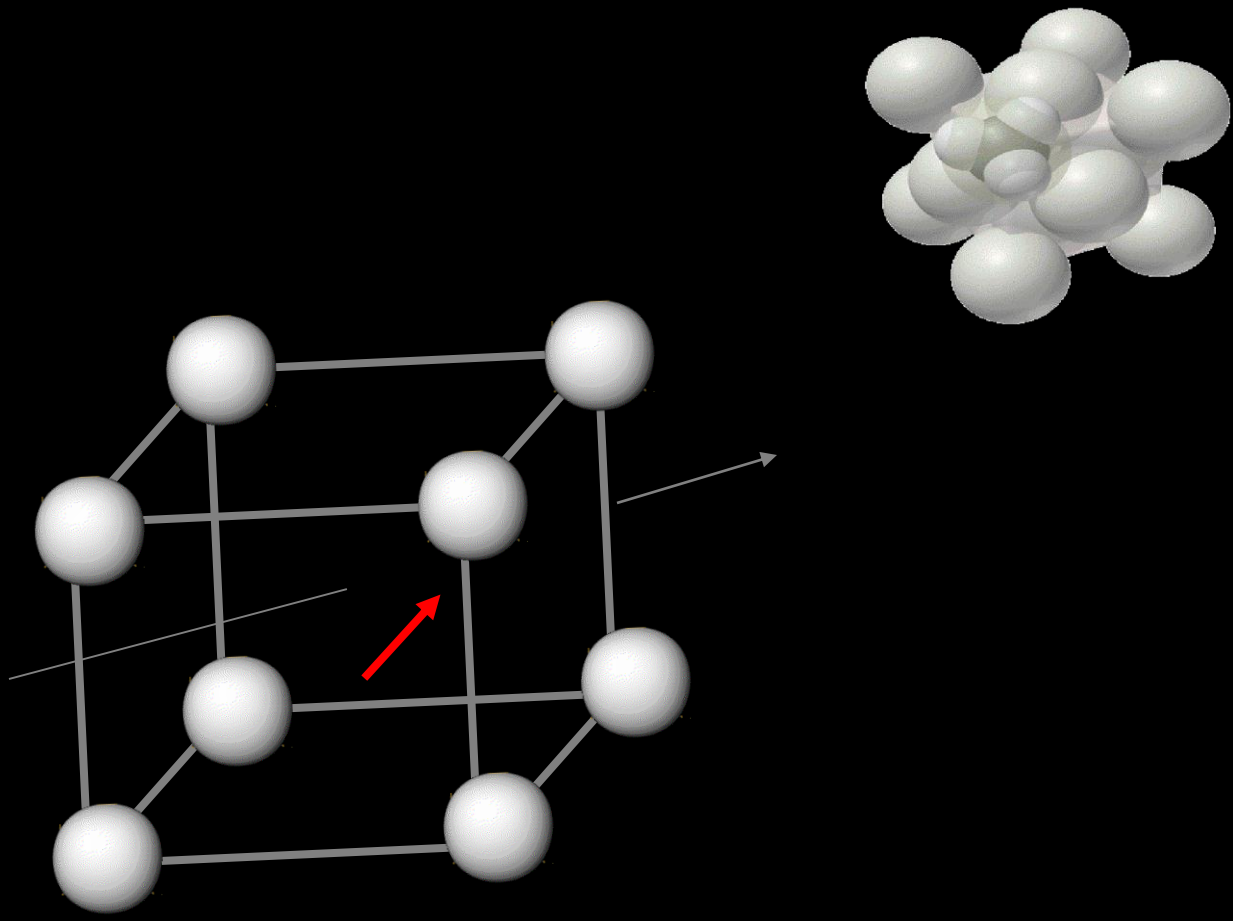
Those arrangements in a given shape that violate even one symmetry element of that shape do not exist in that shape

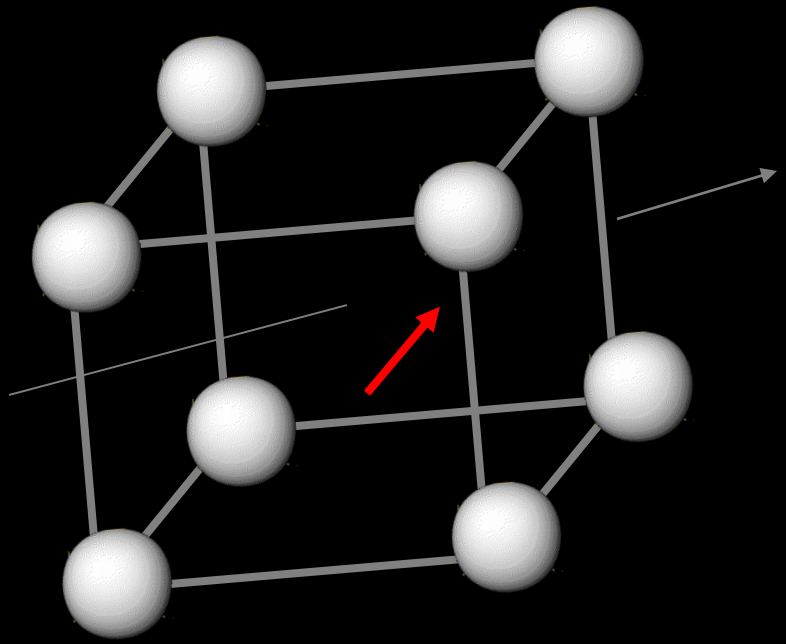
90º axis of symmetry

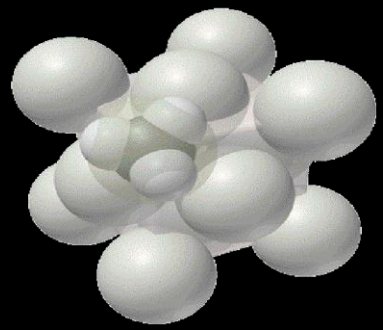


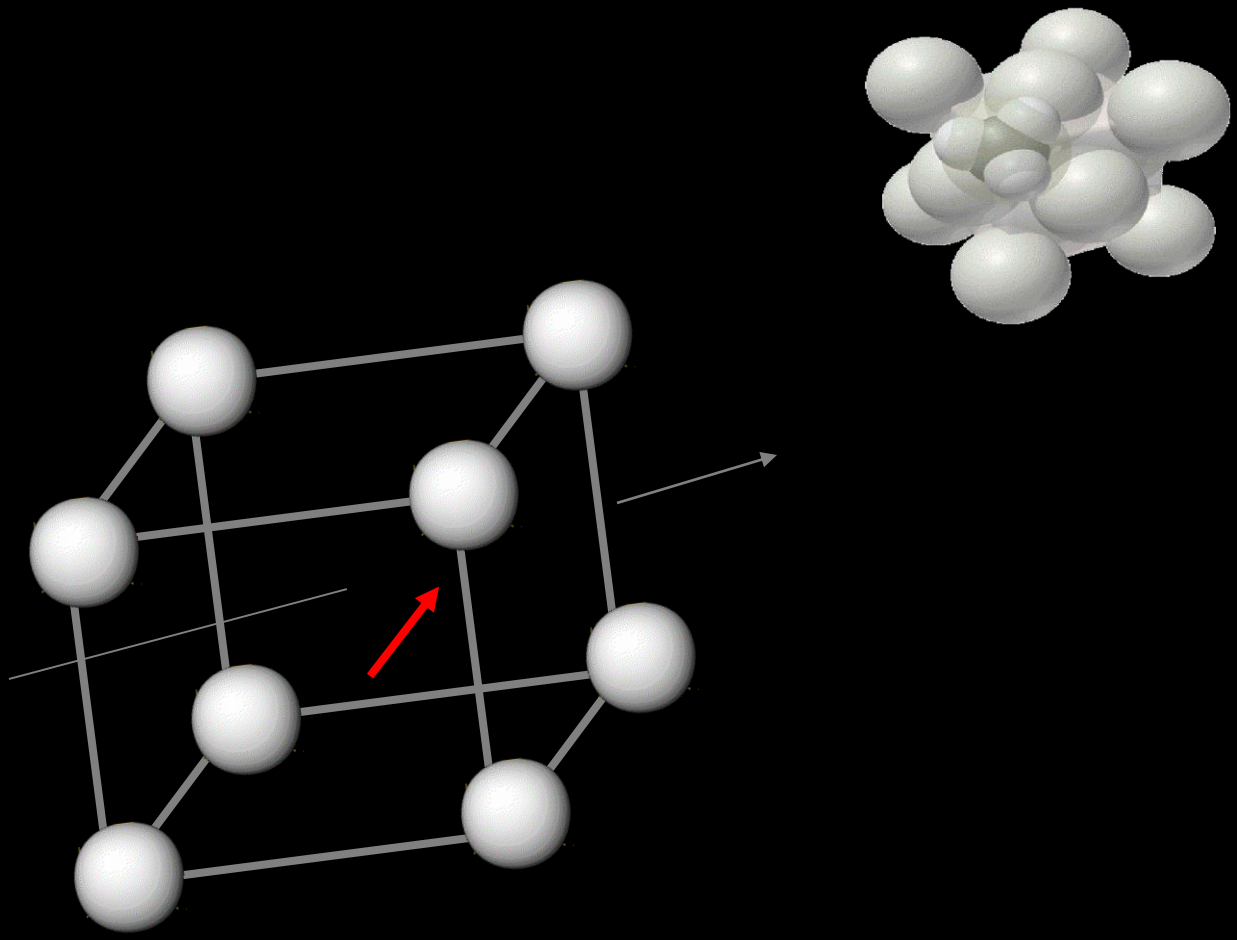


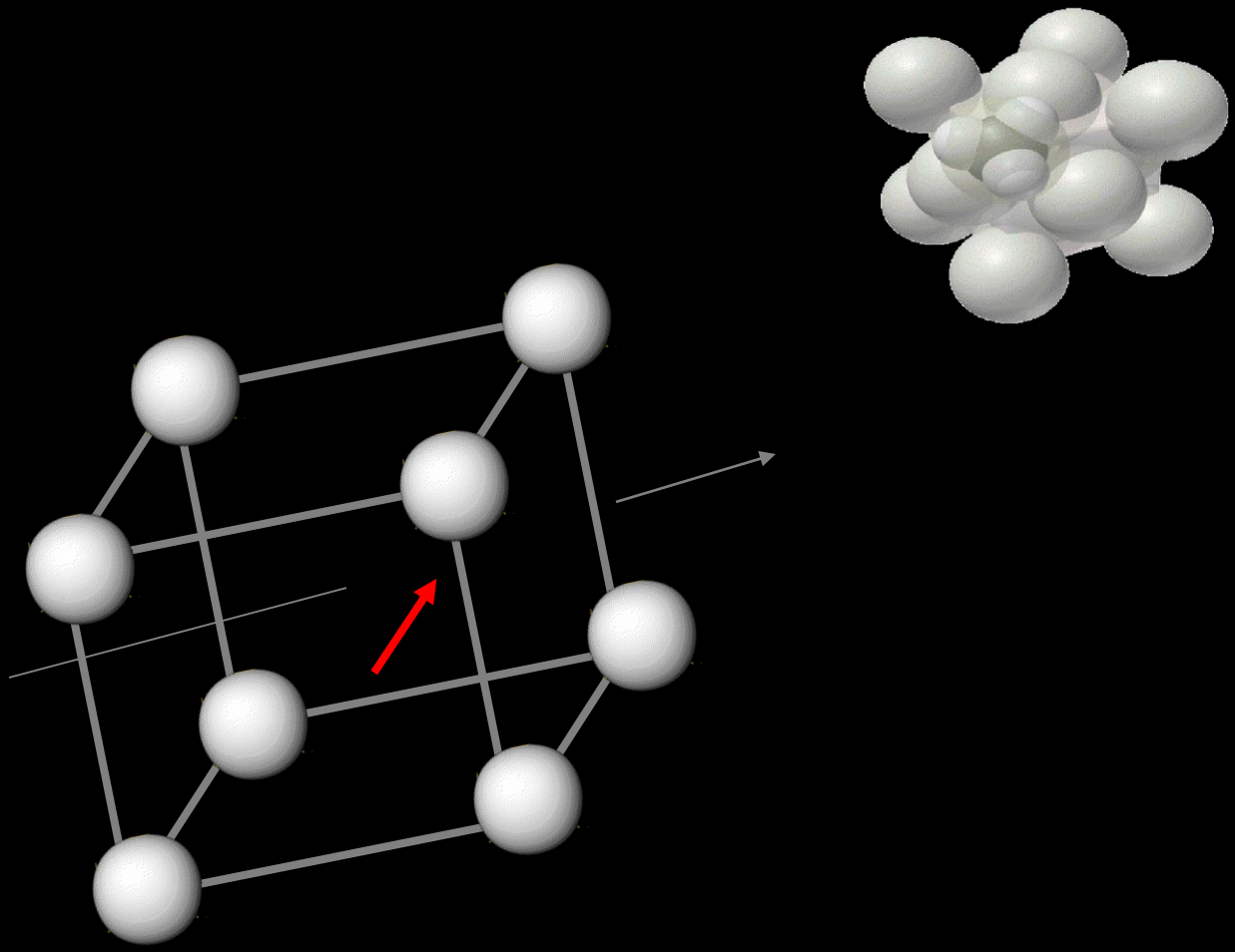


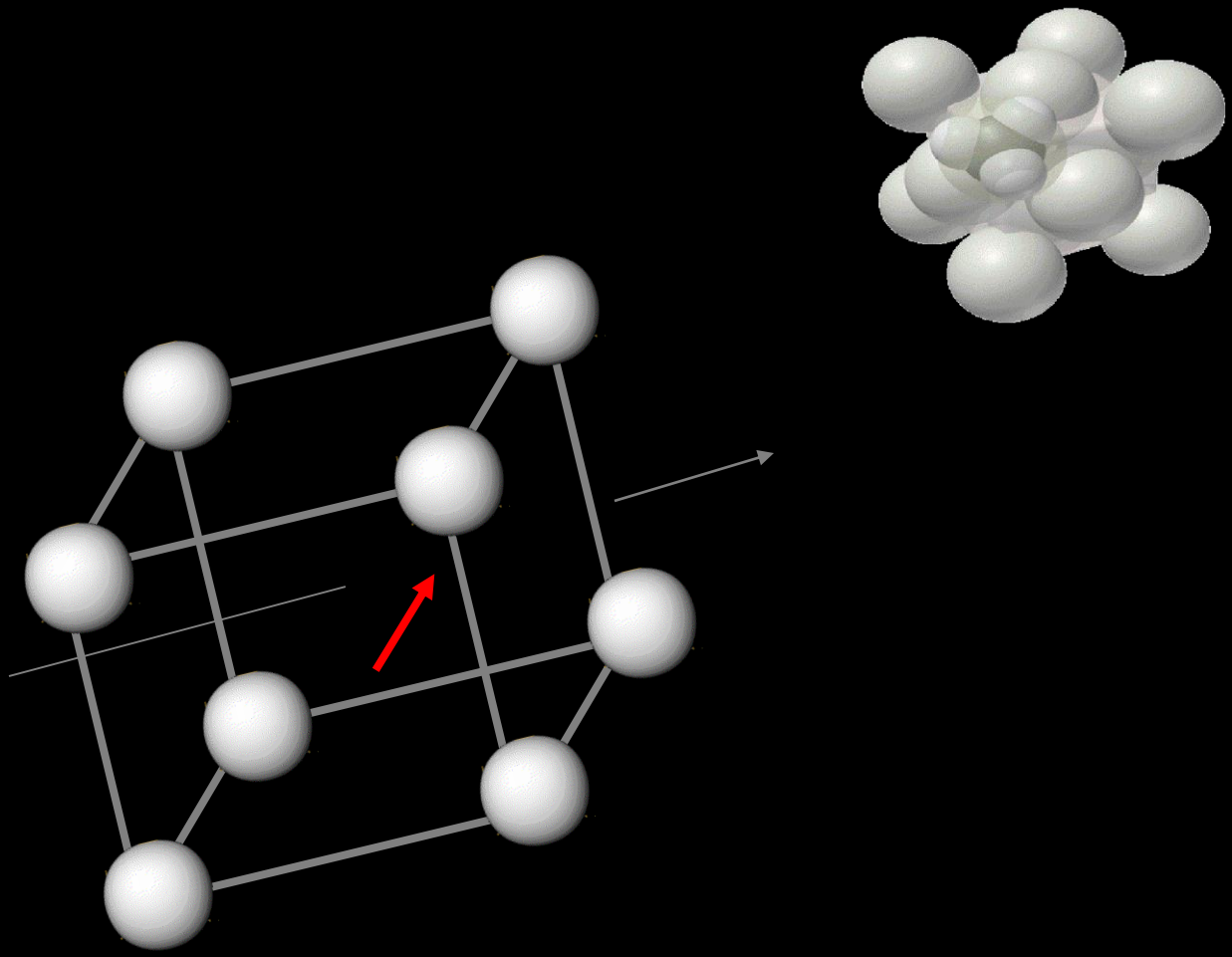


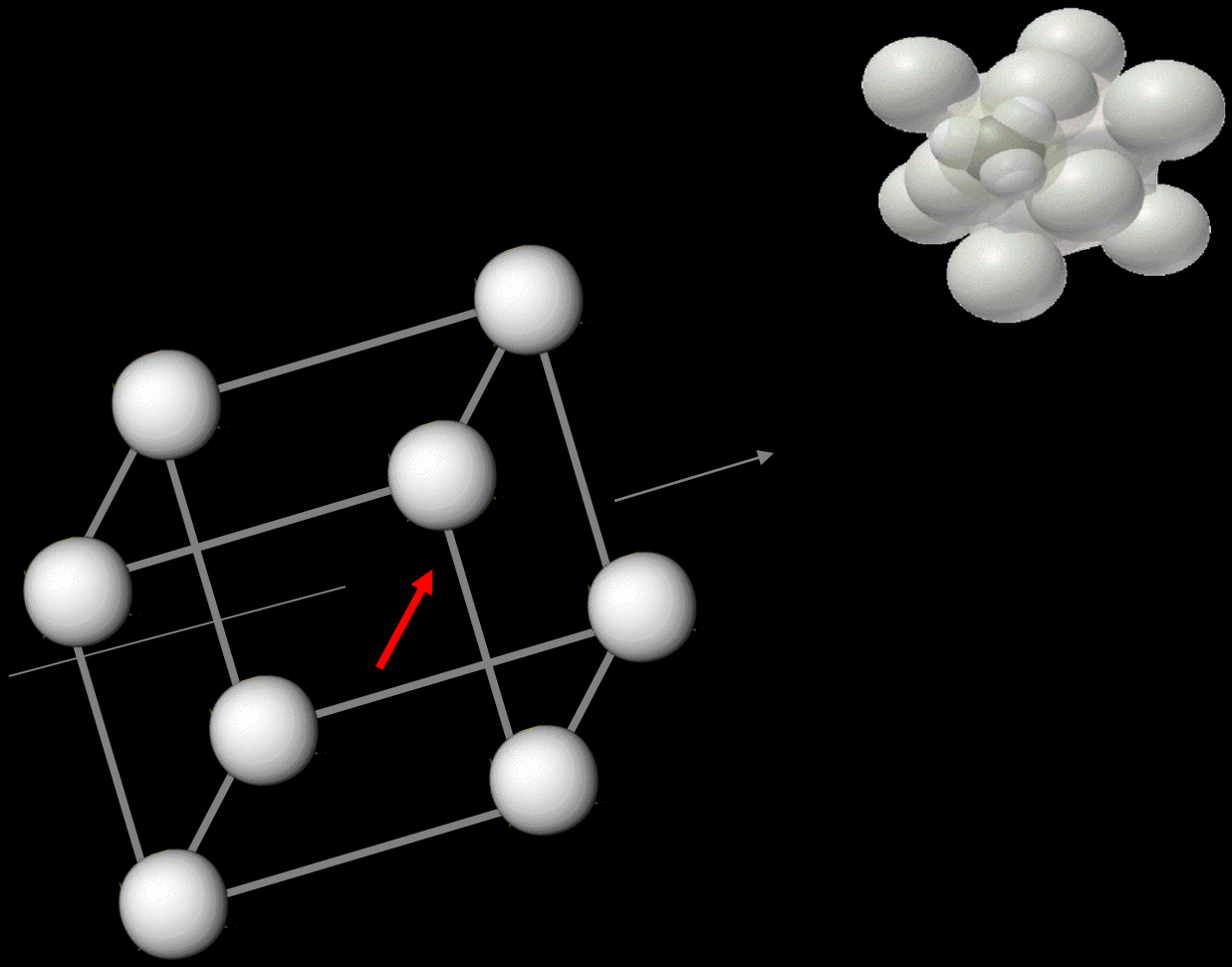


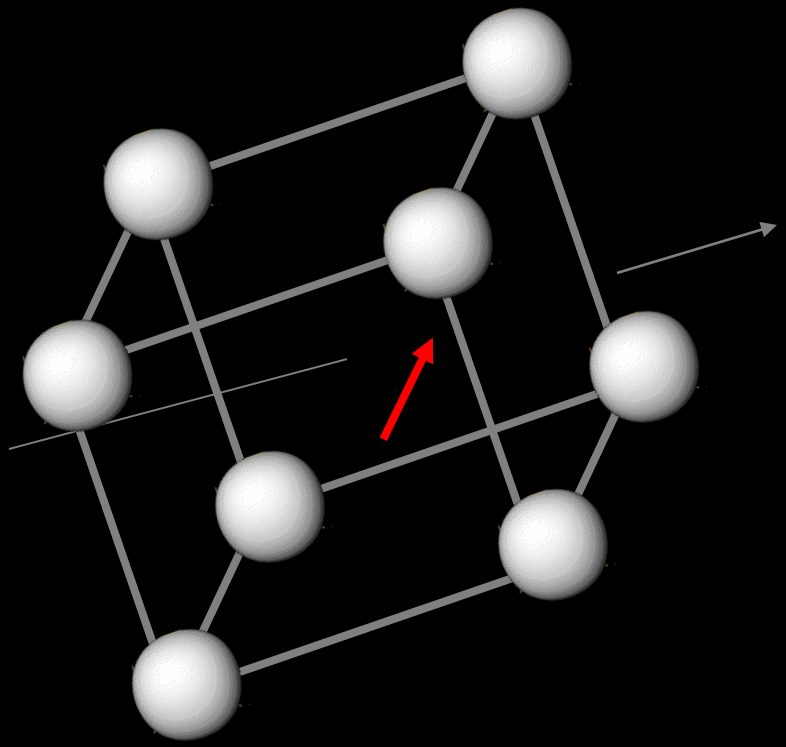


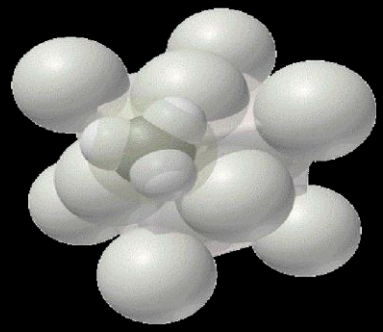


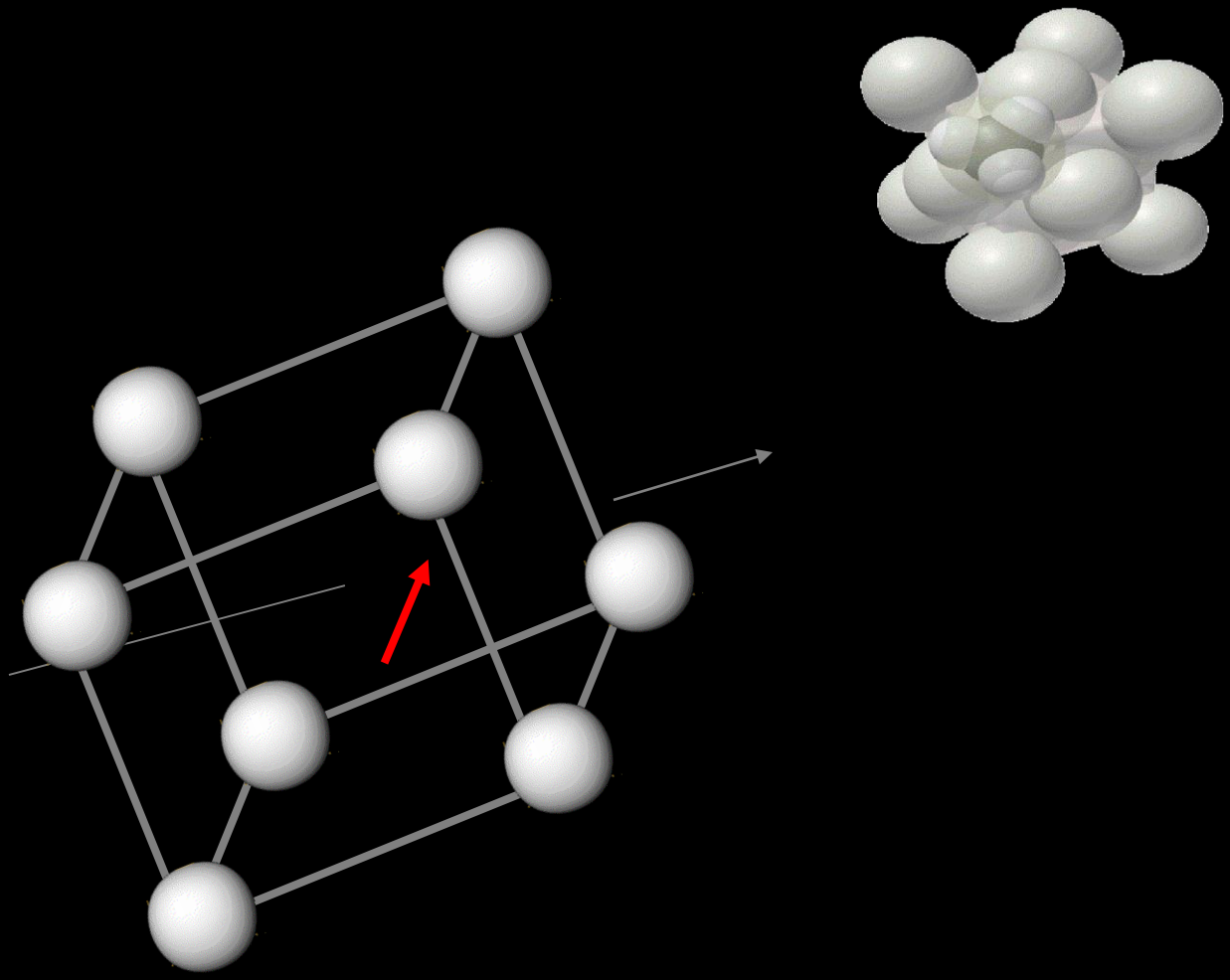


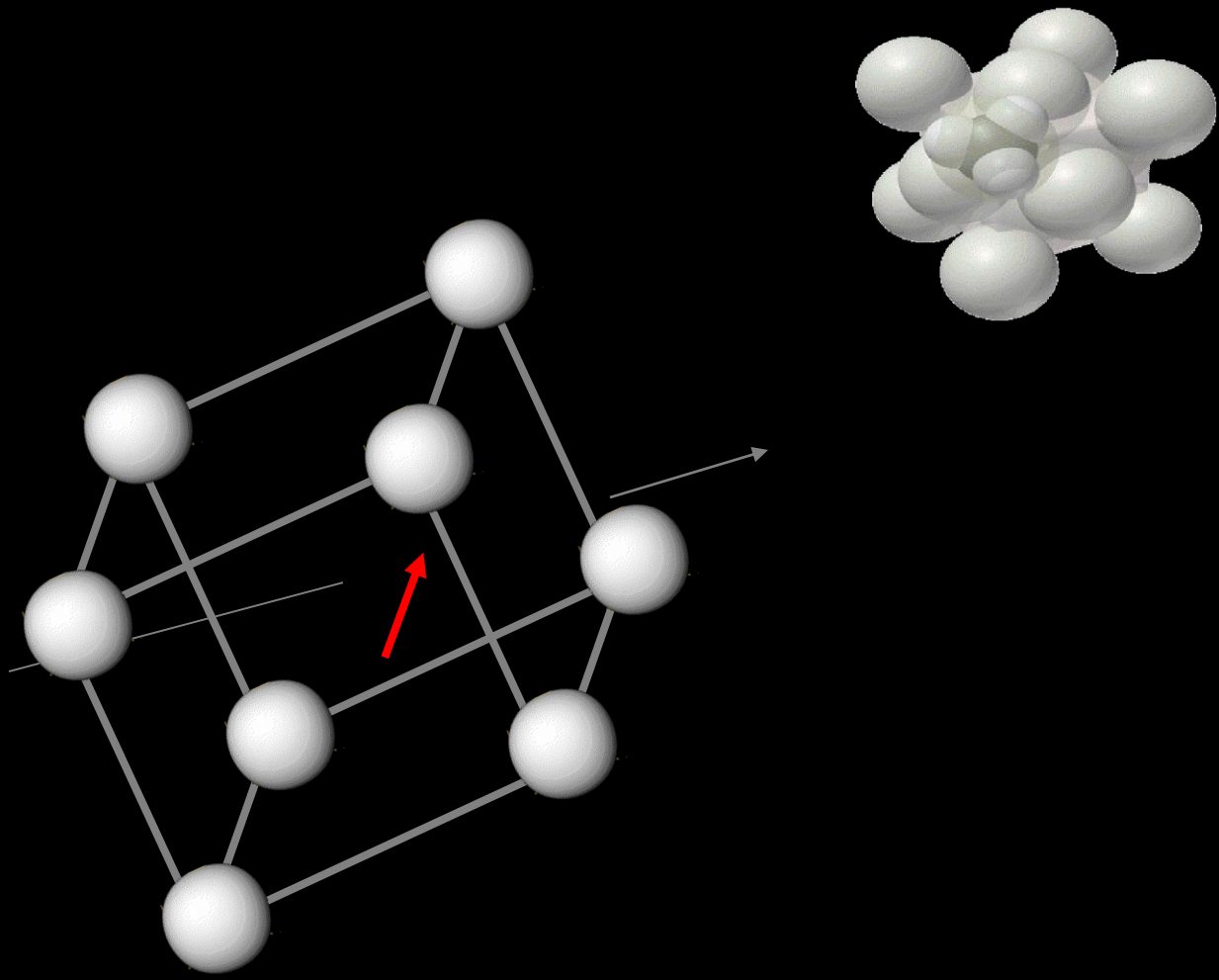


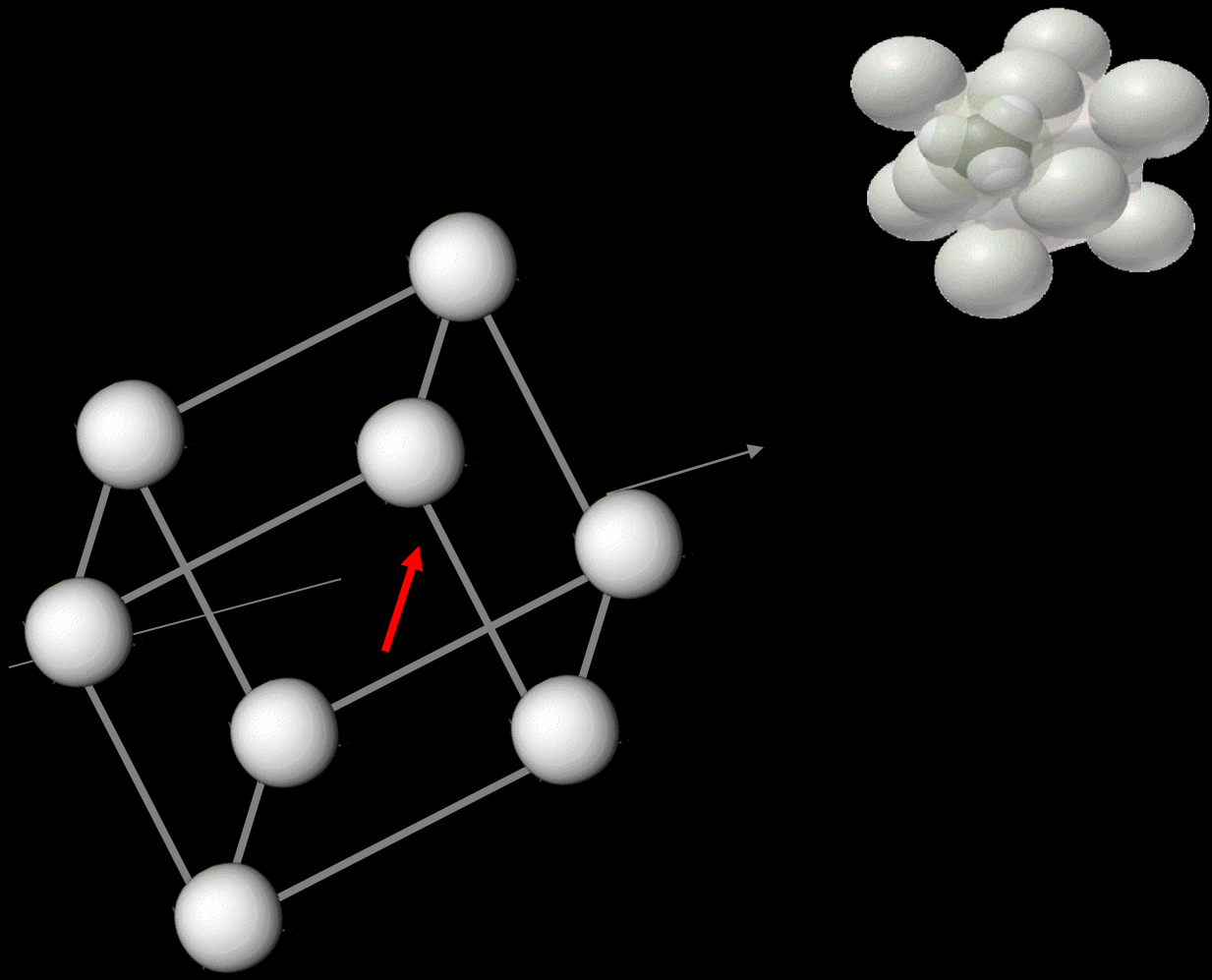


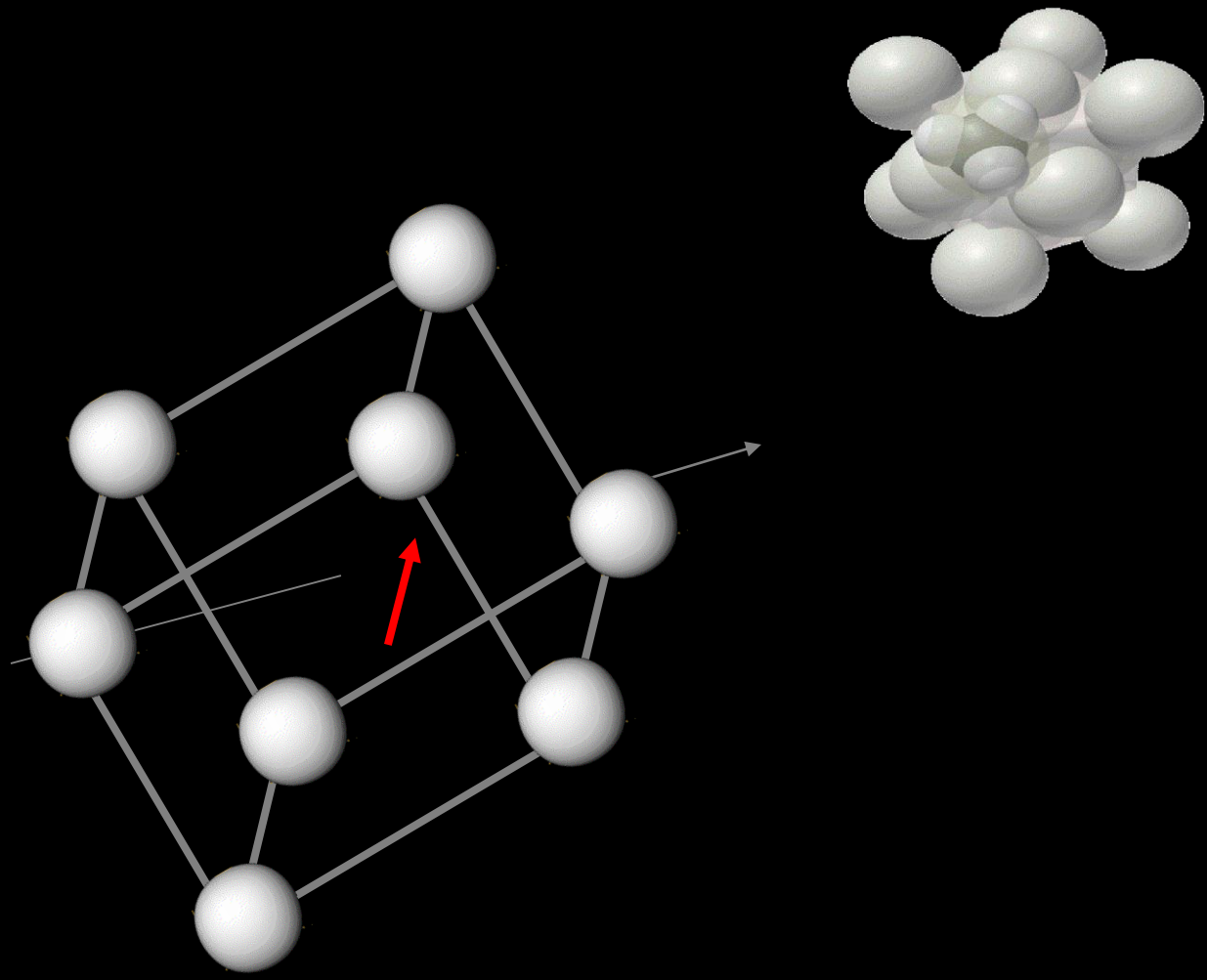


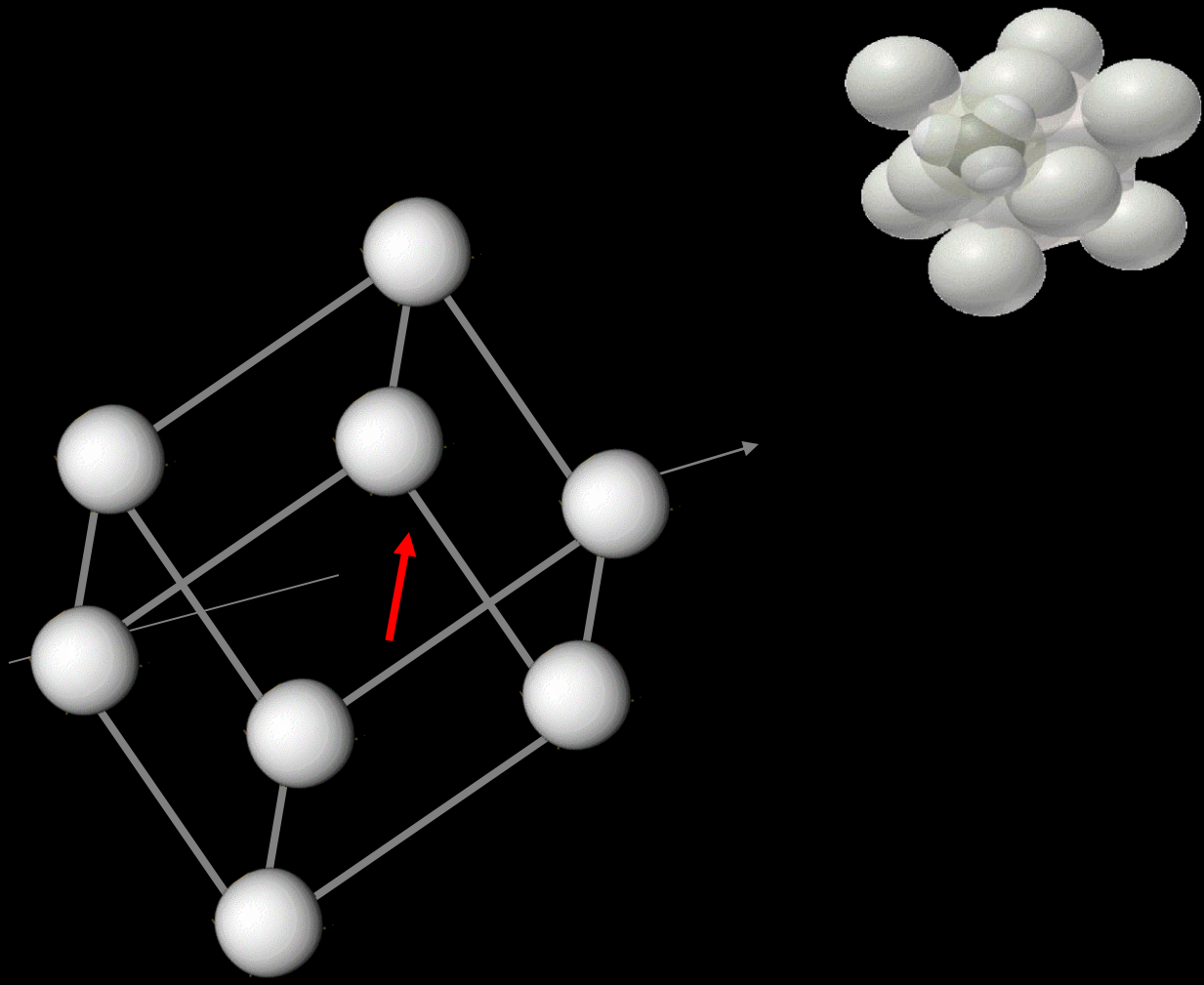


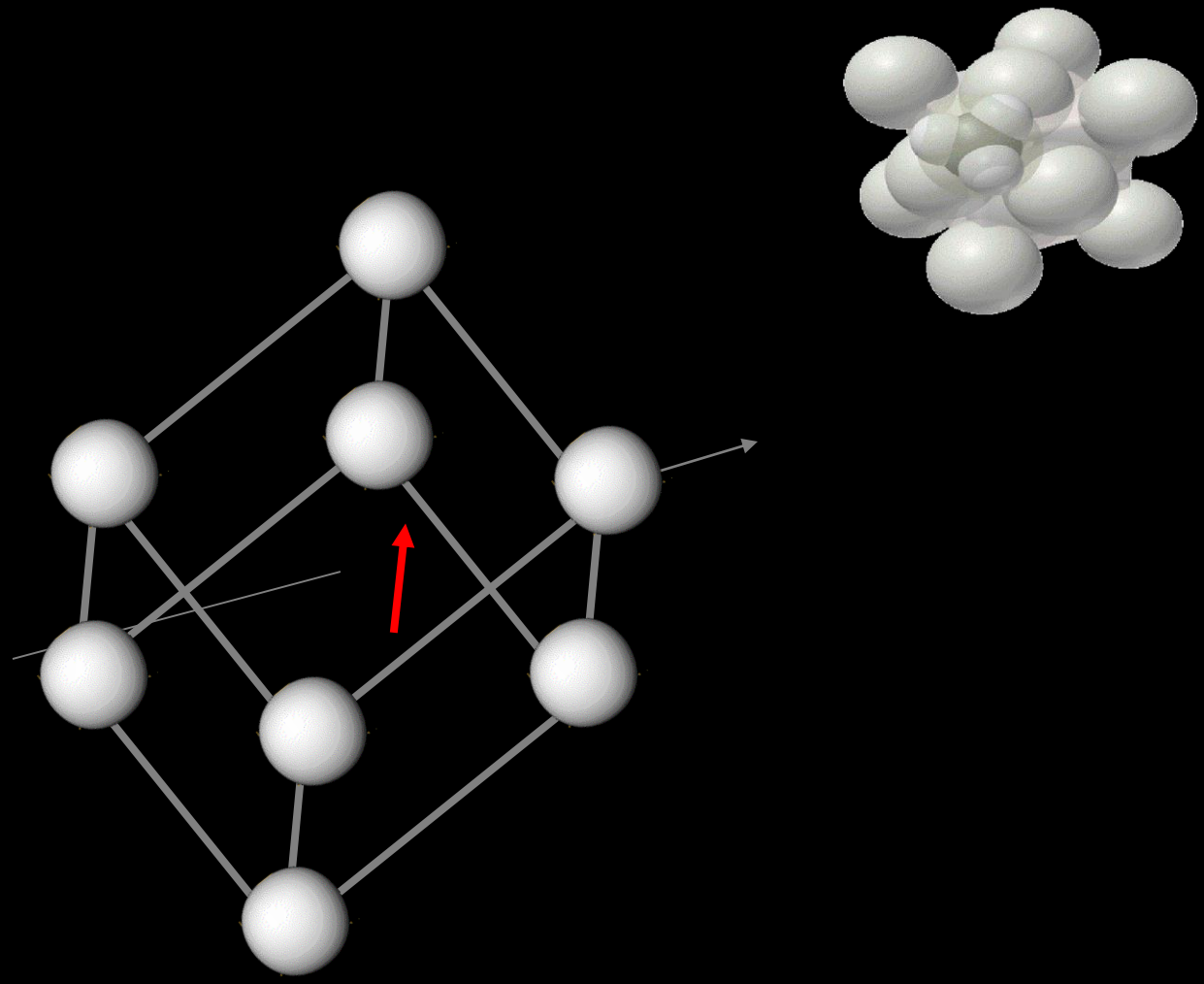


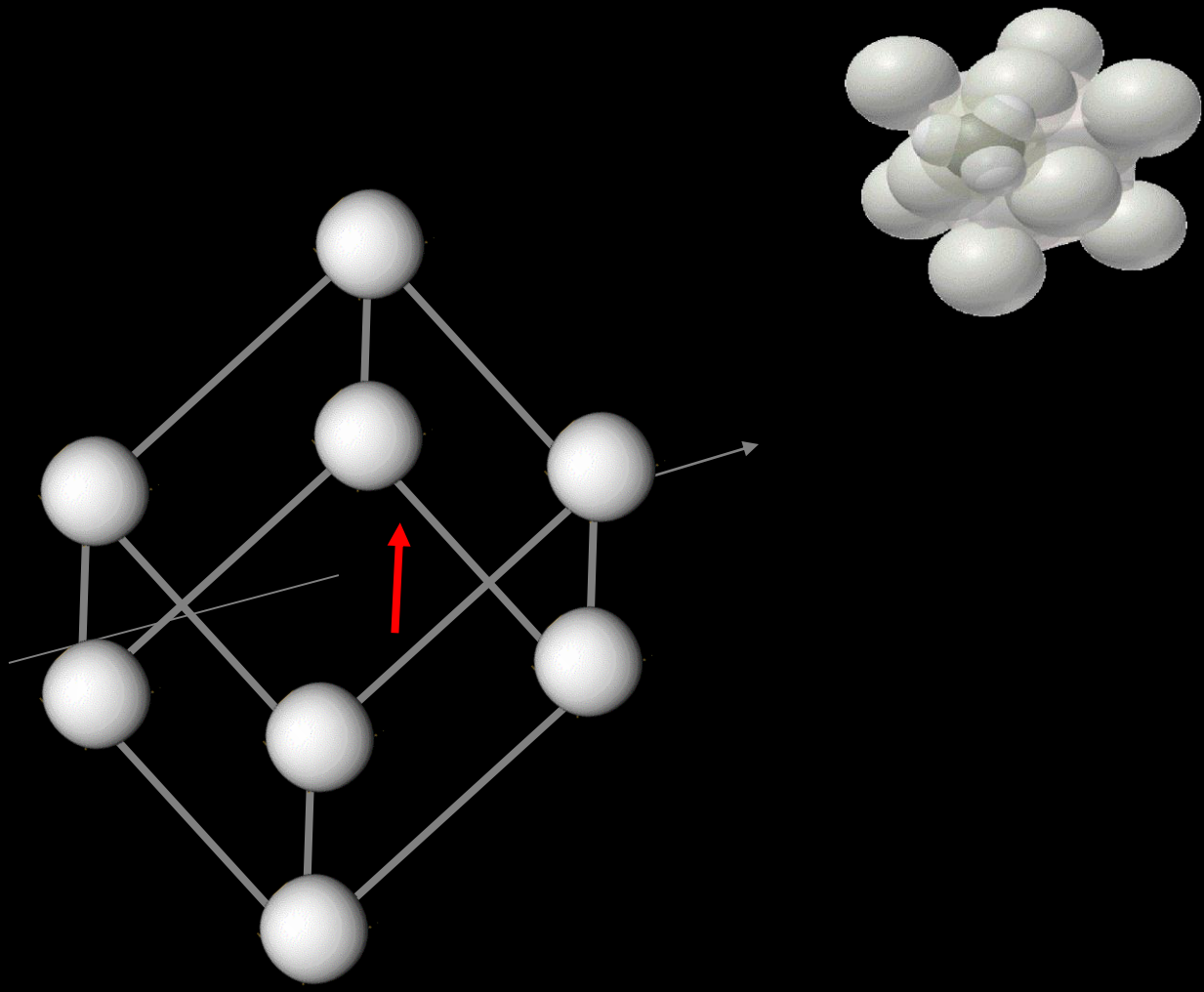


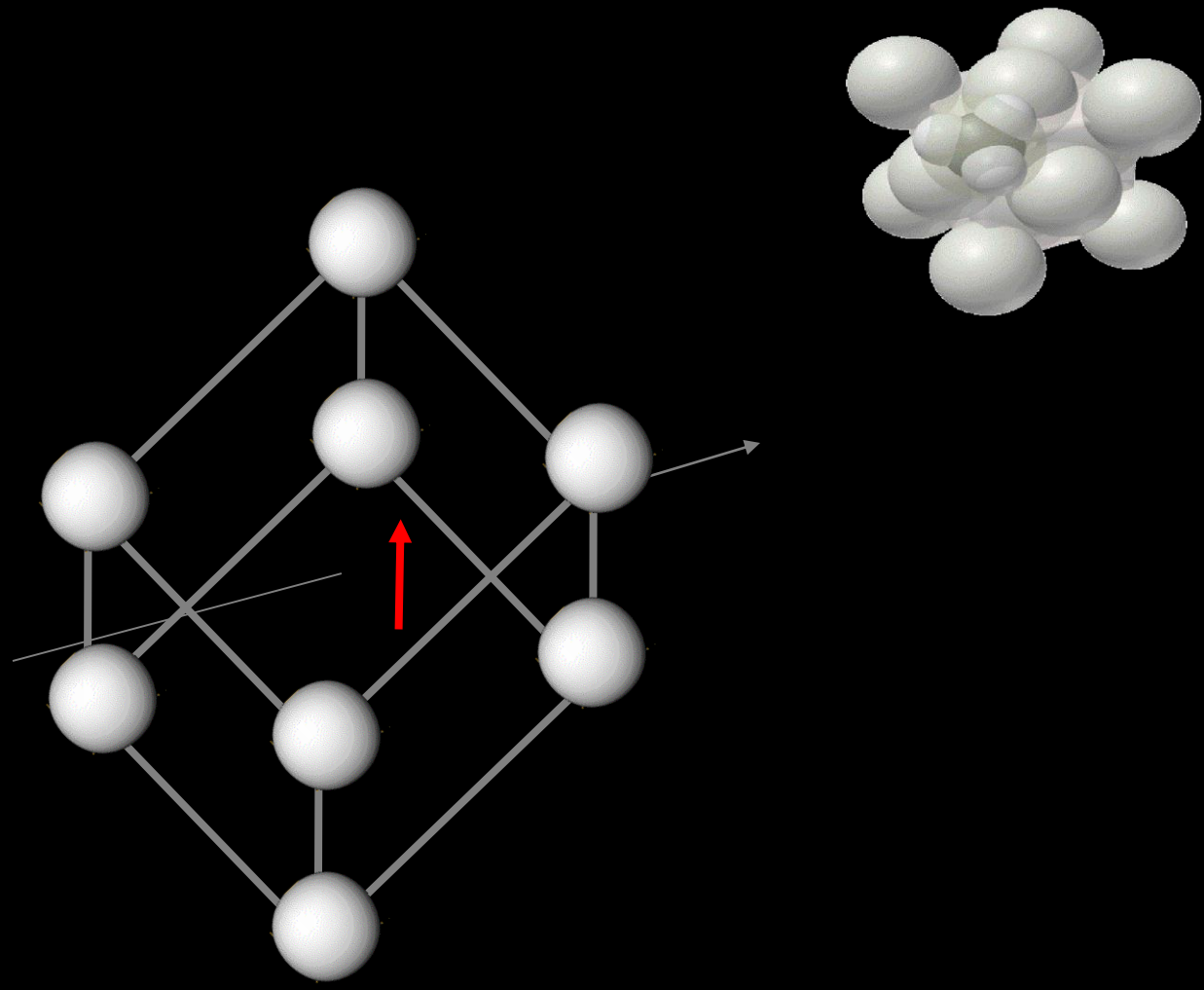


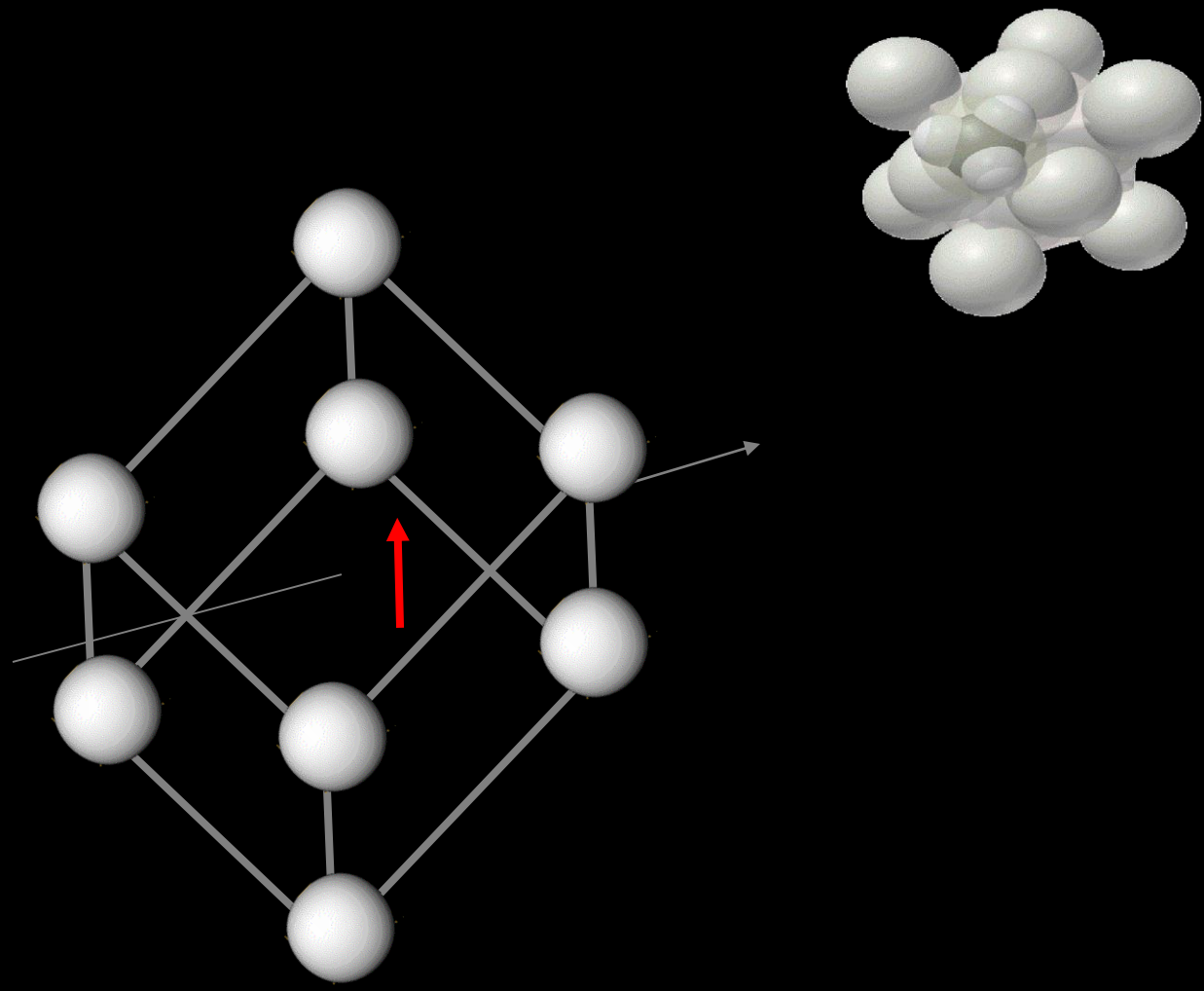


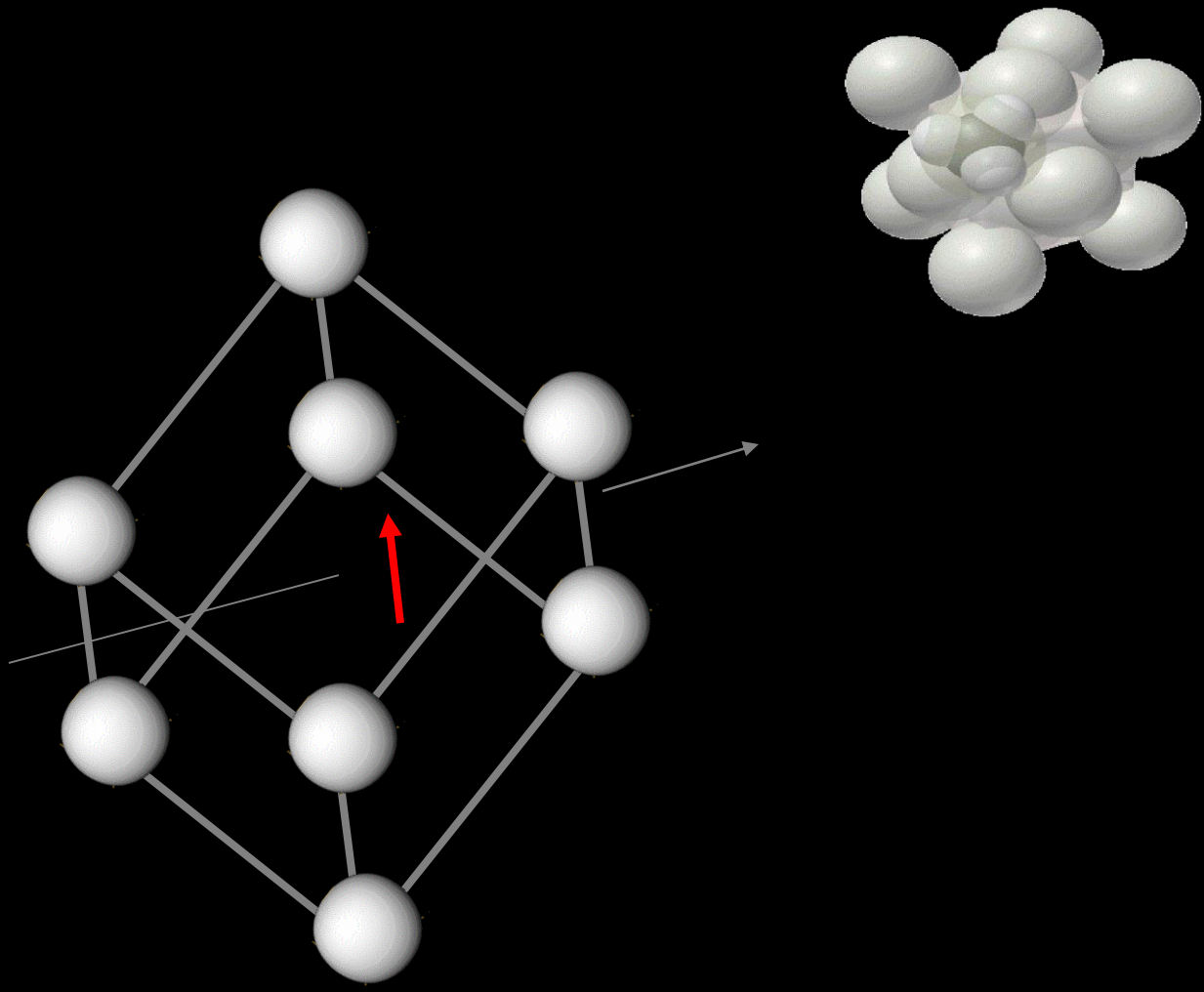


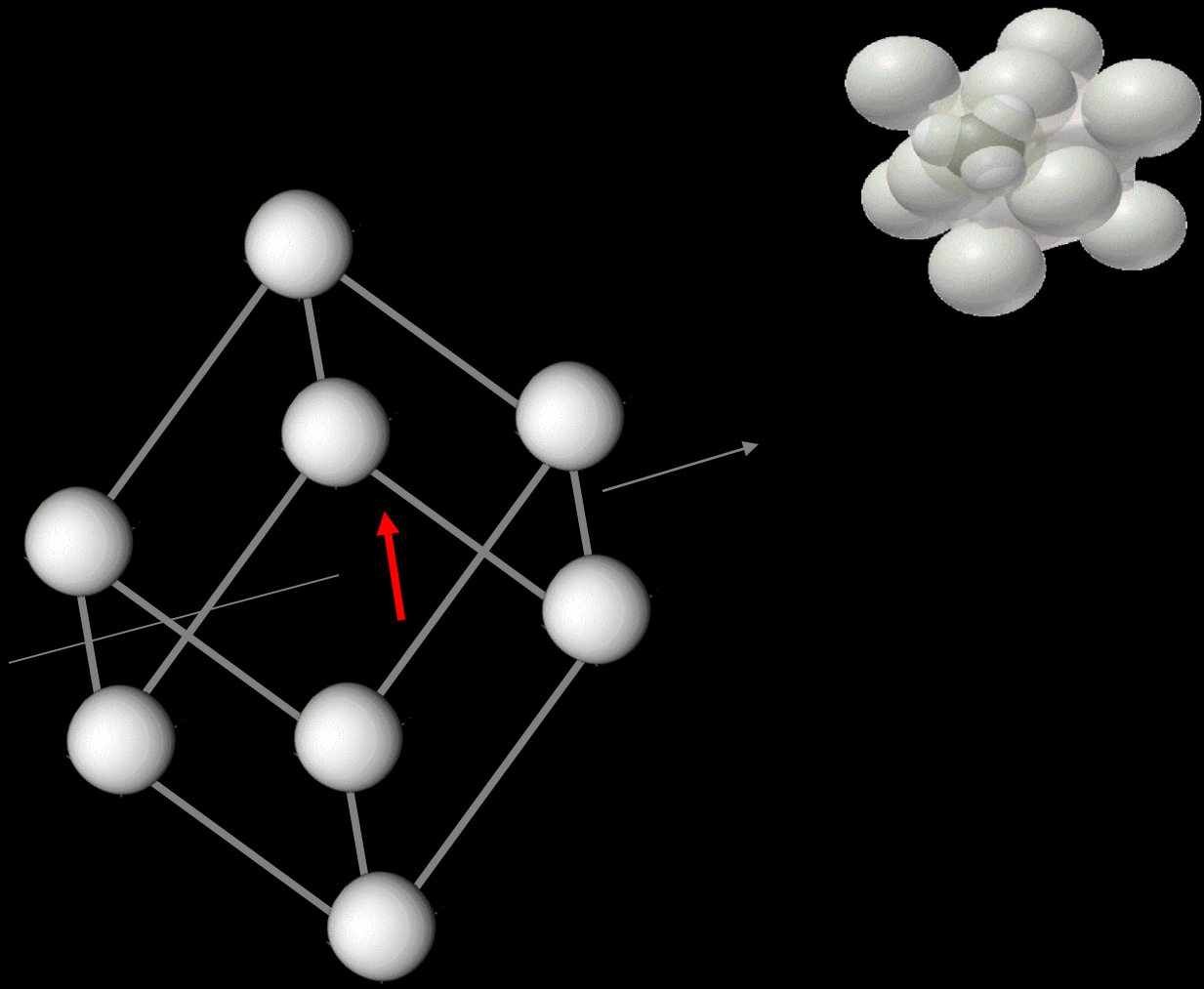


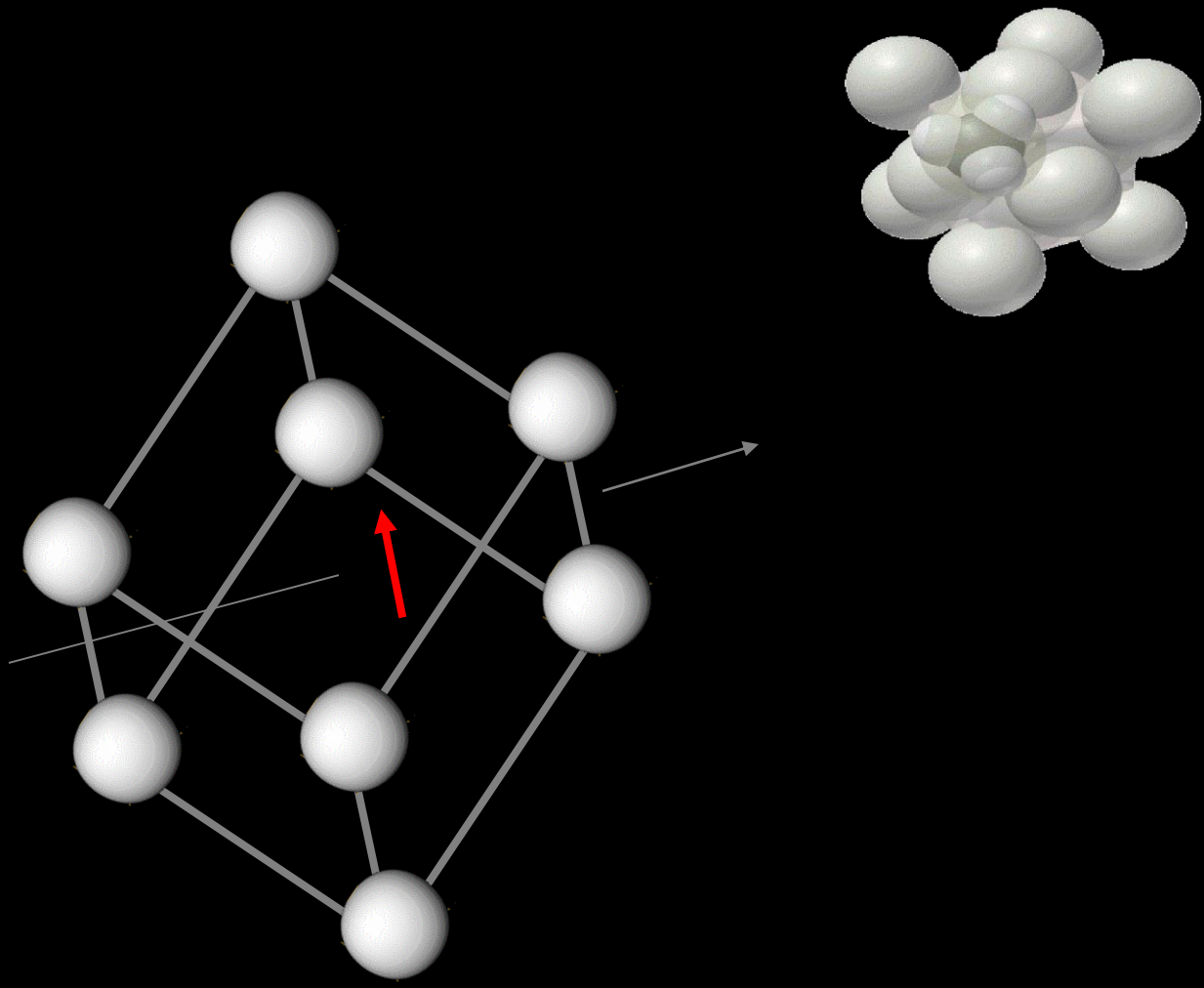


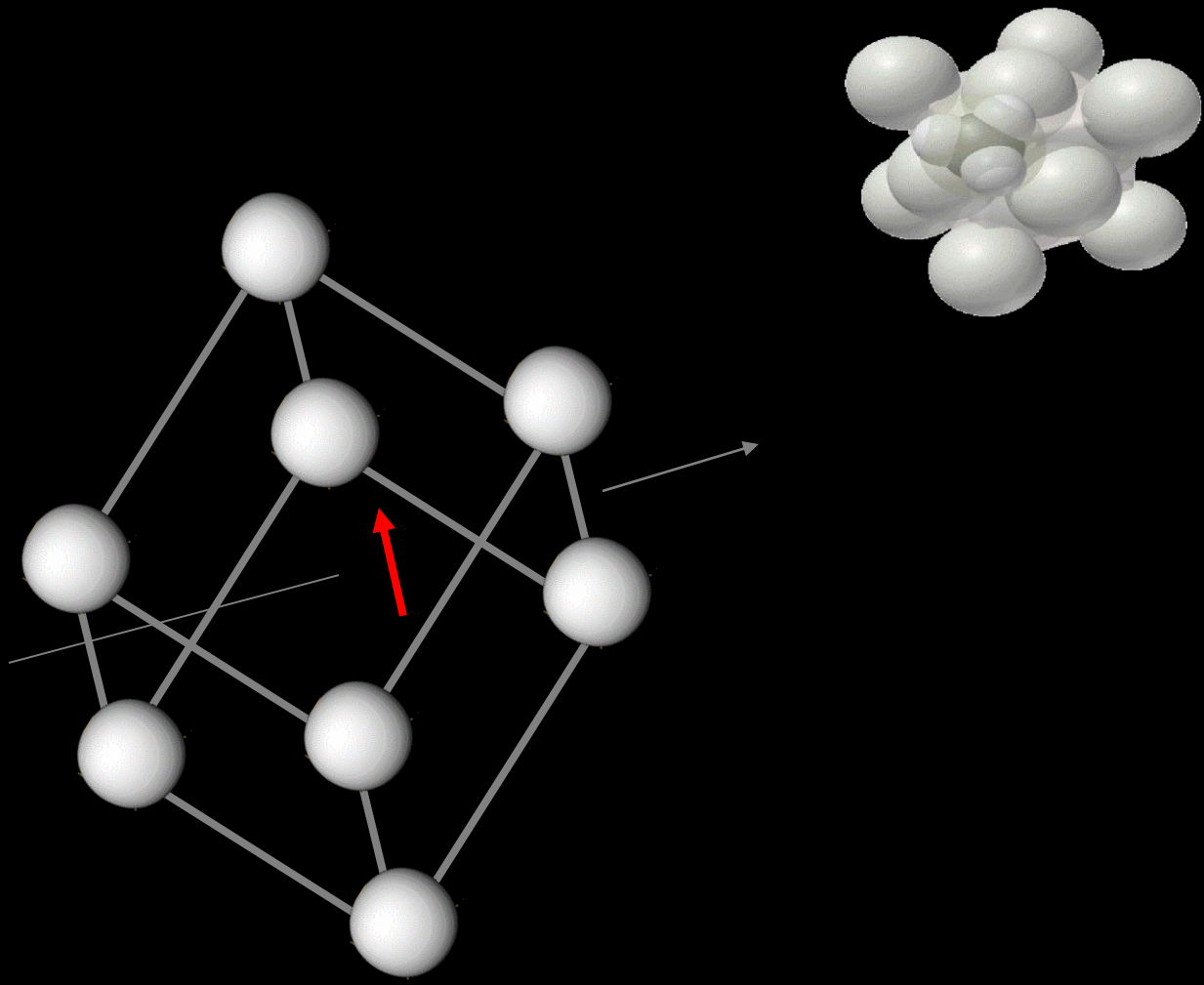


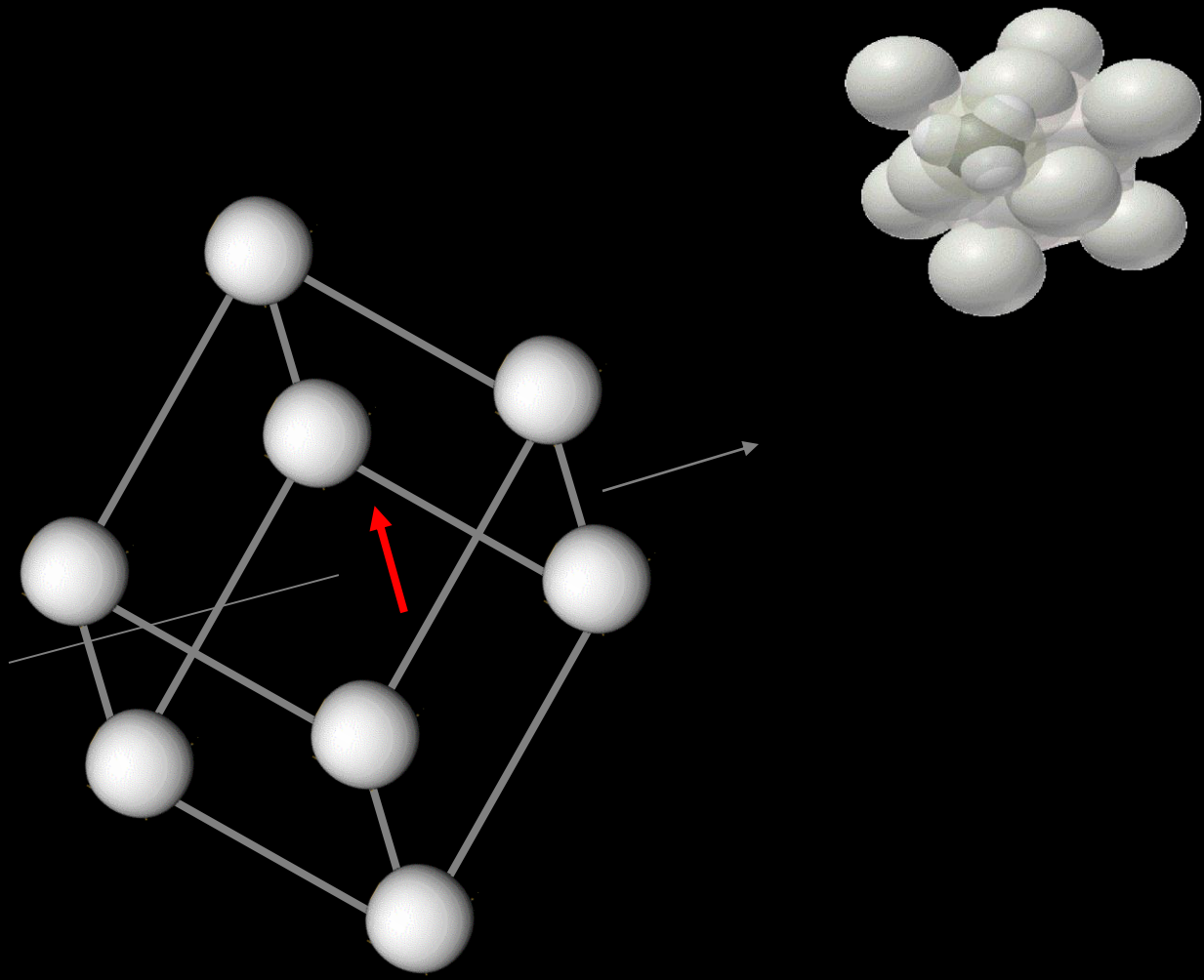


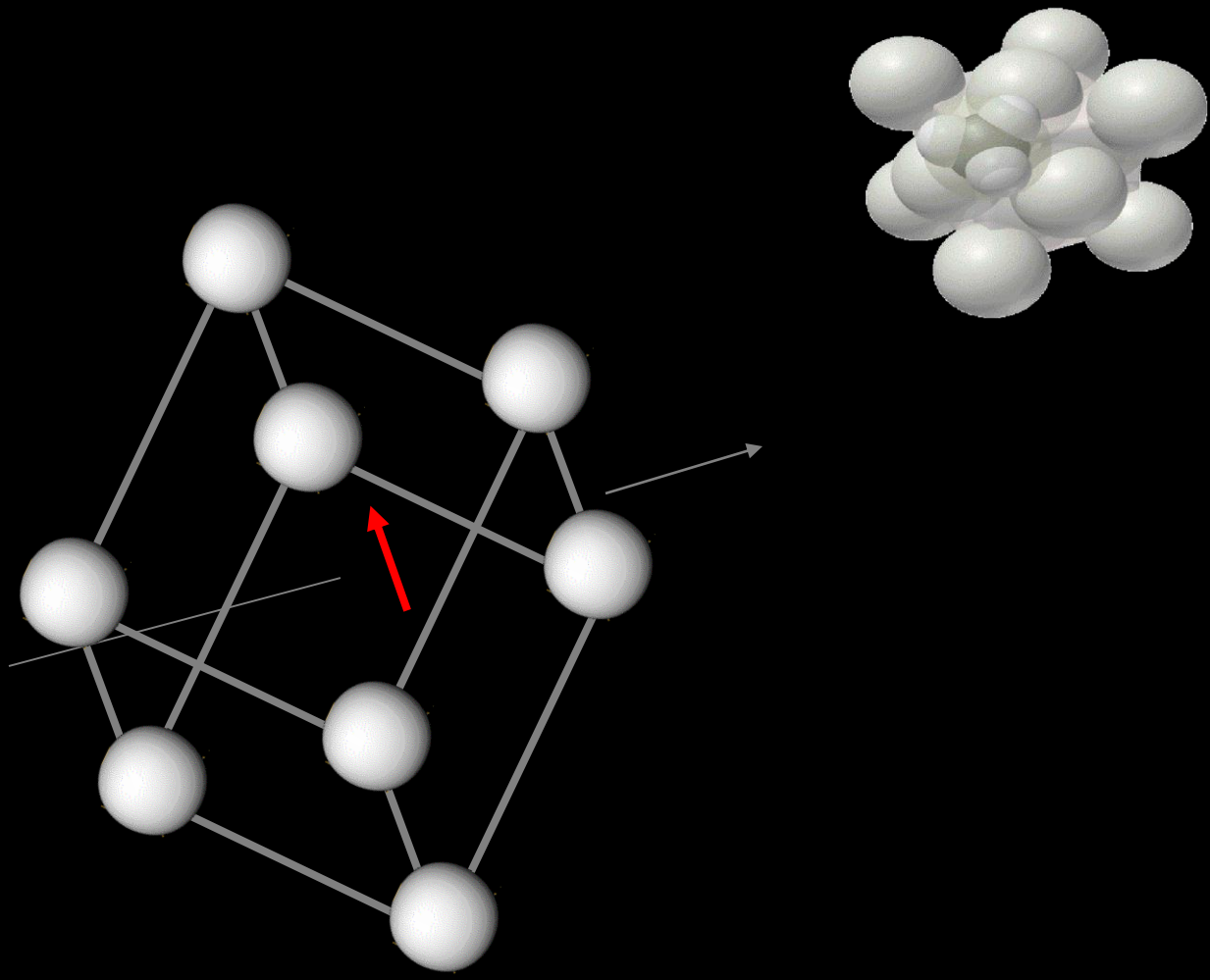


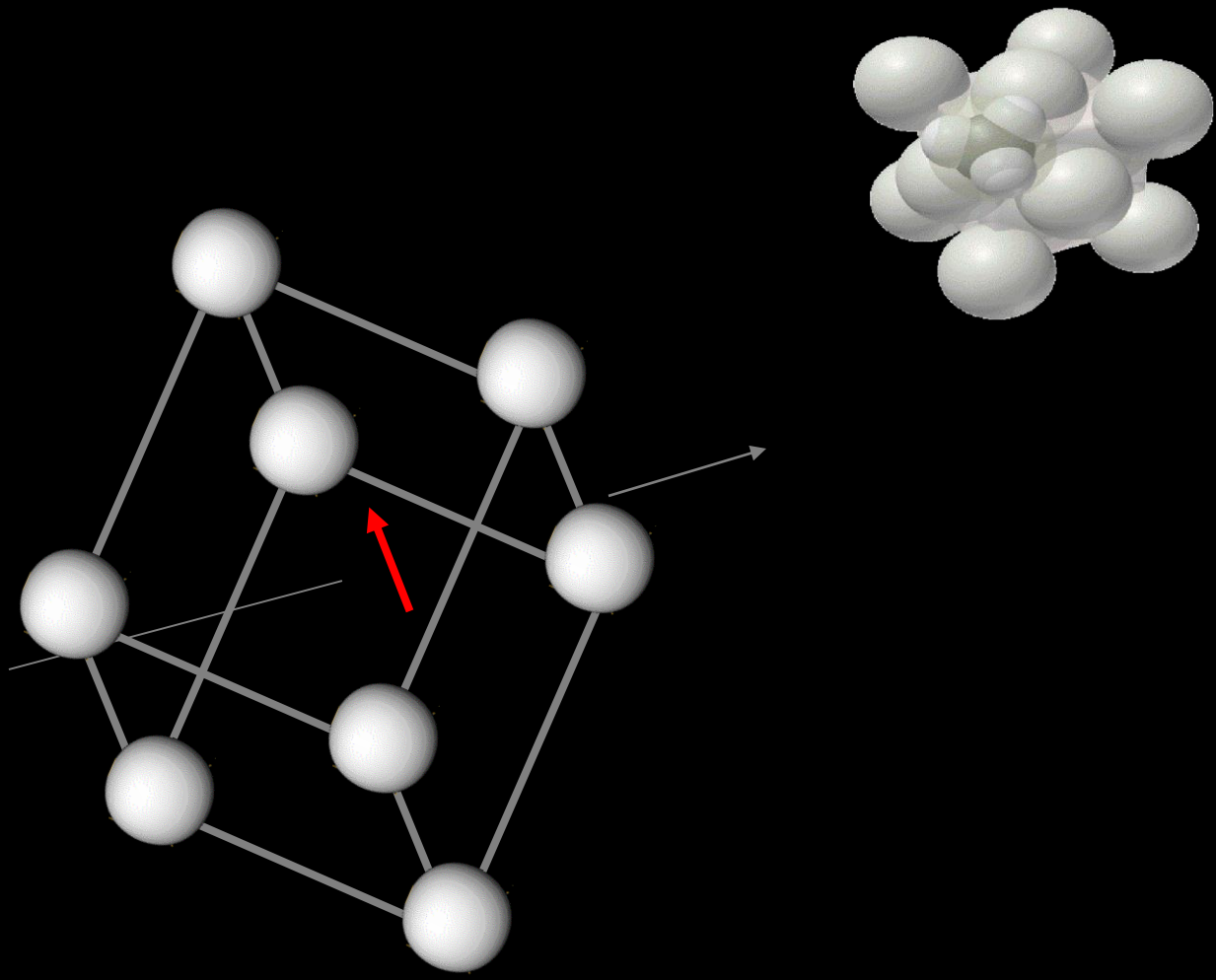


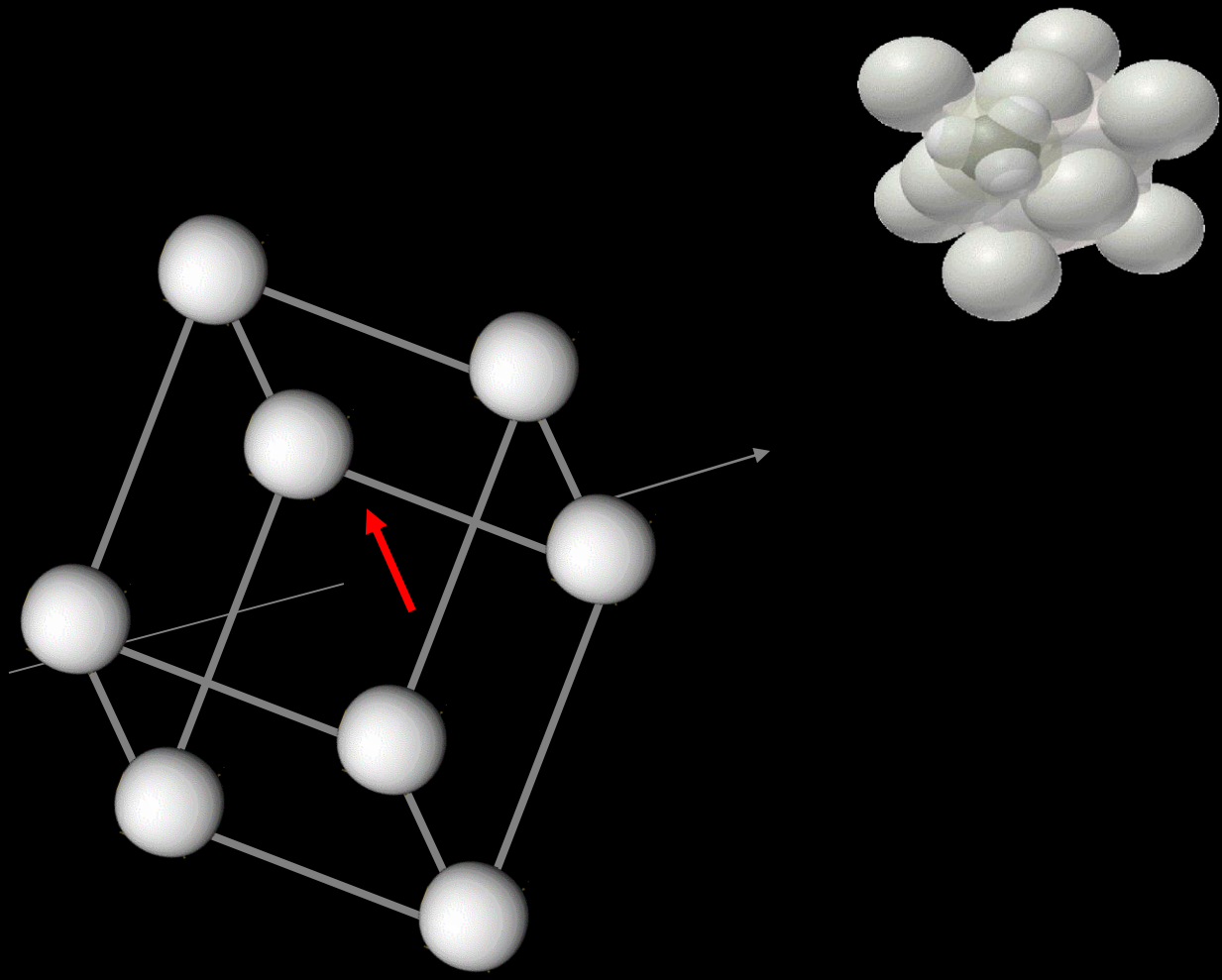


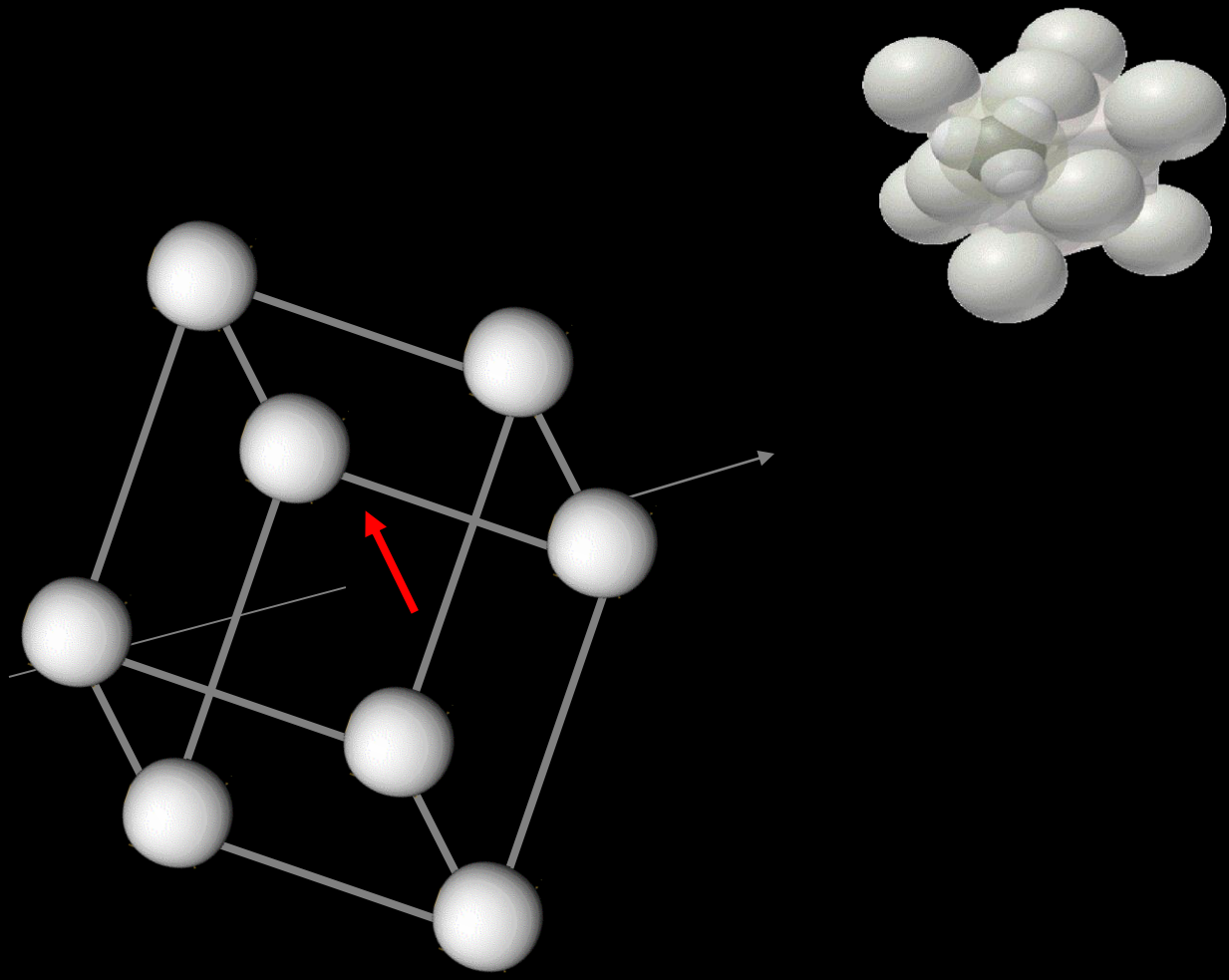


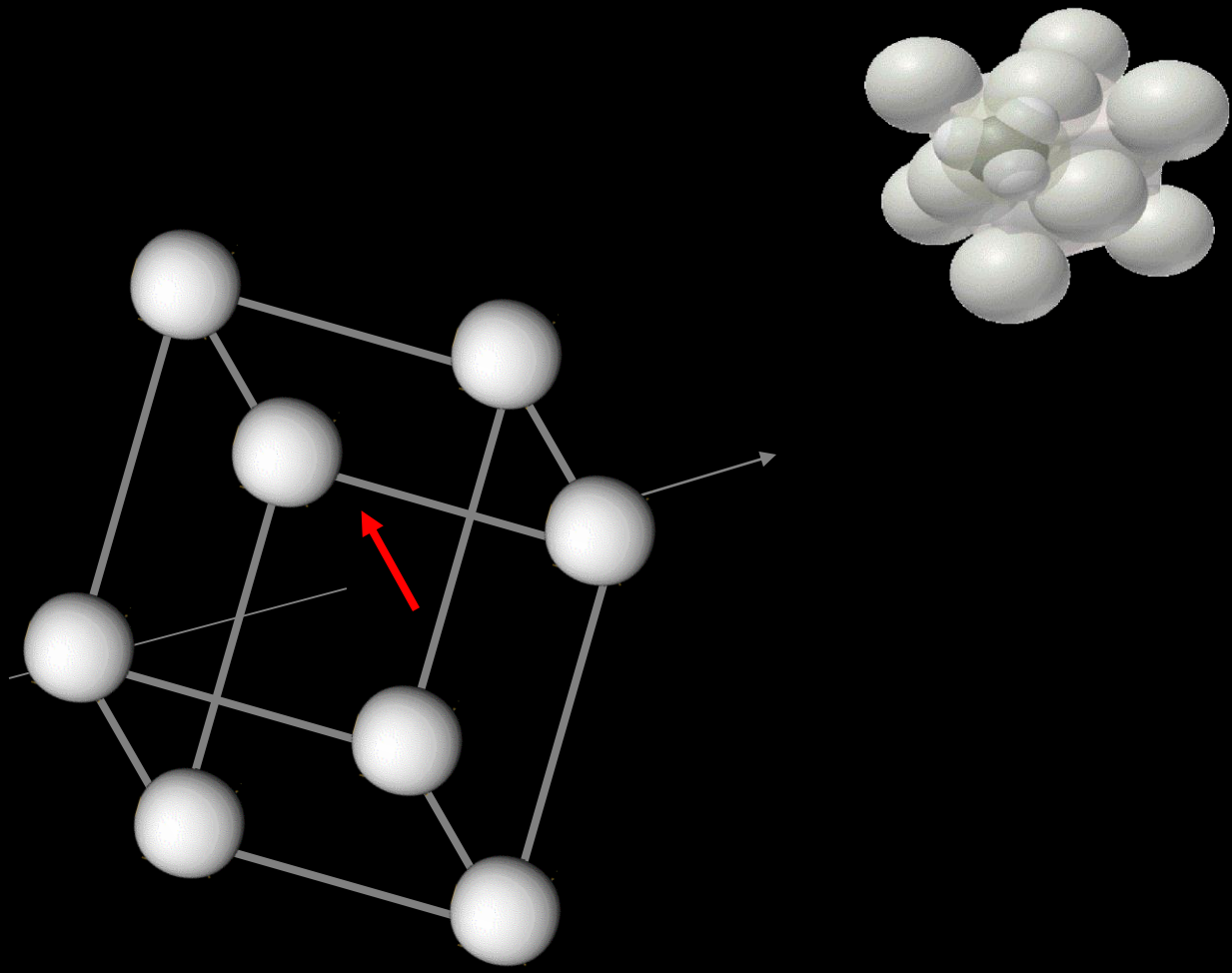


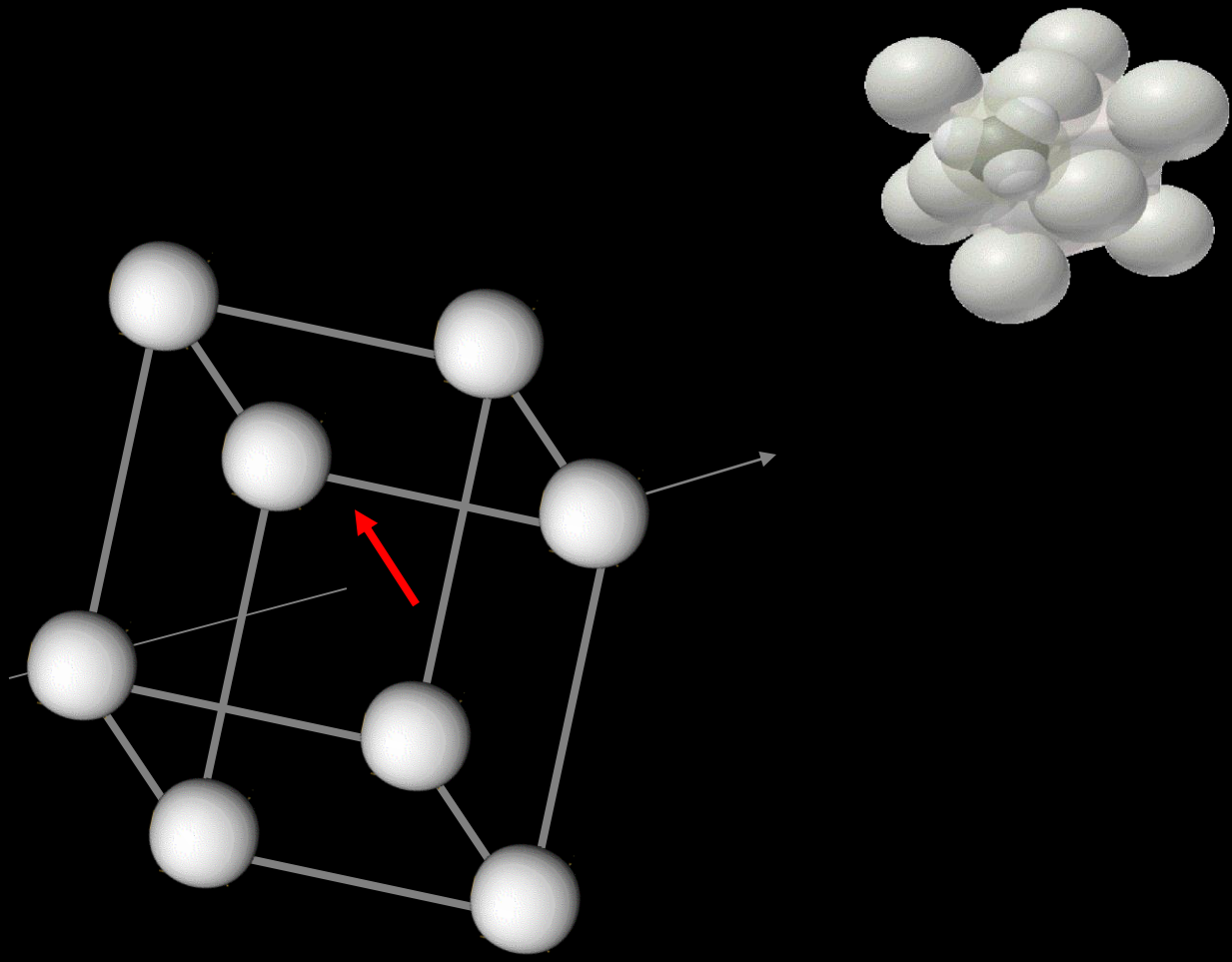


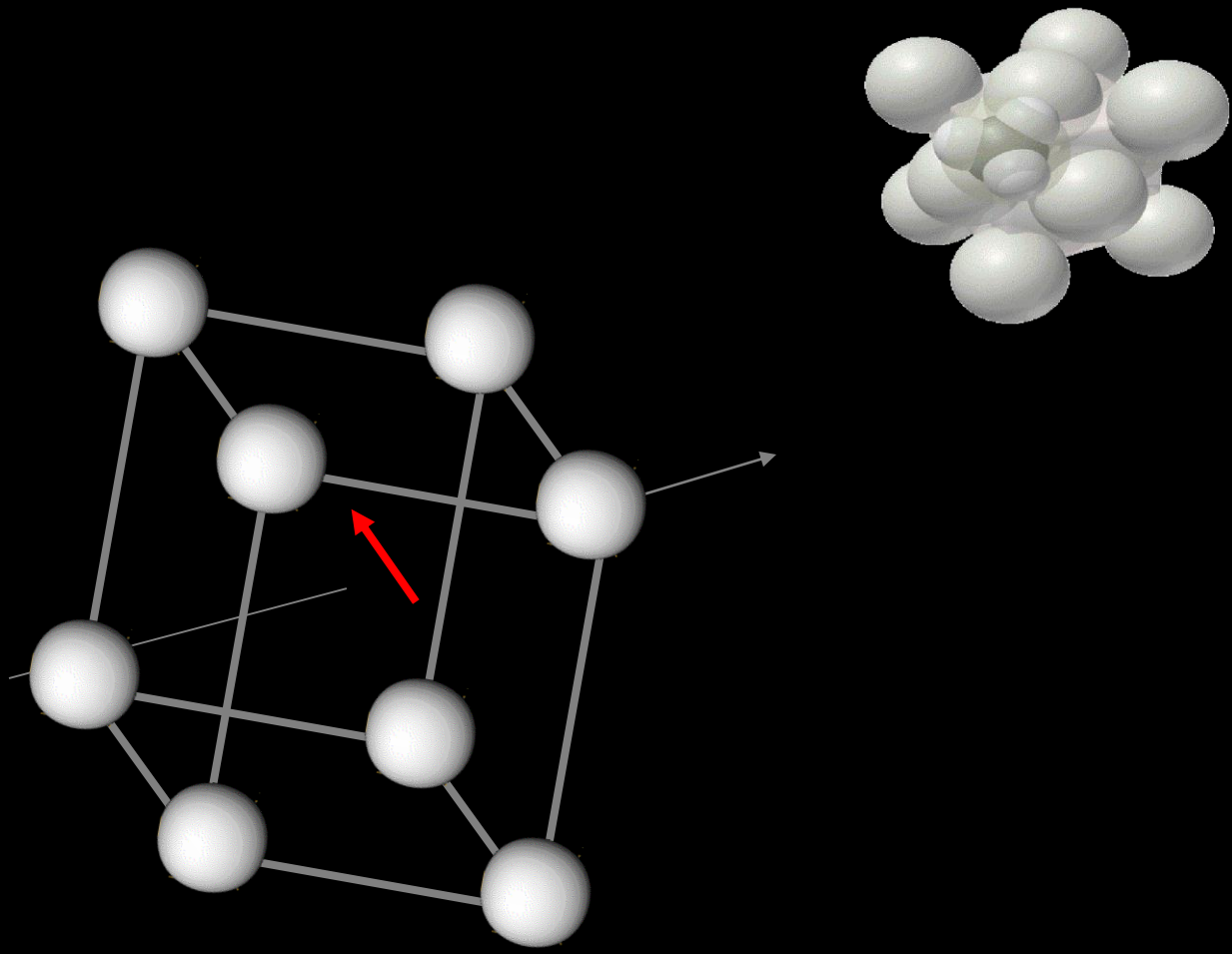


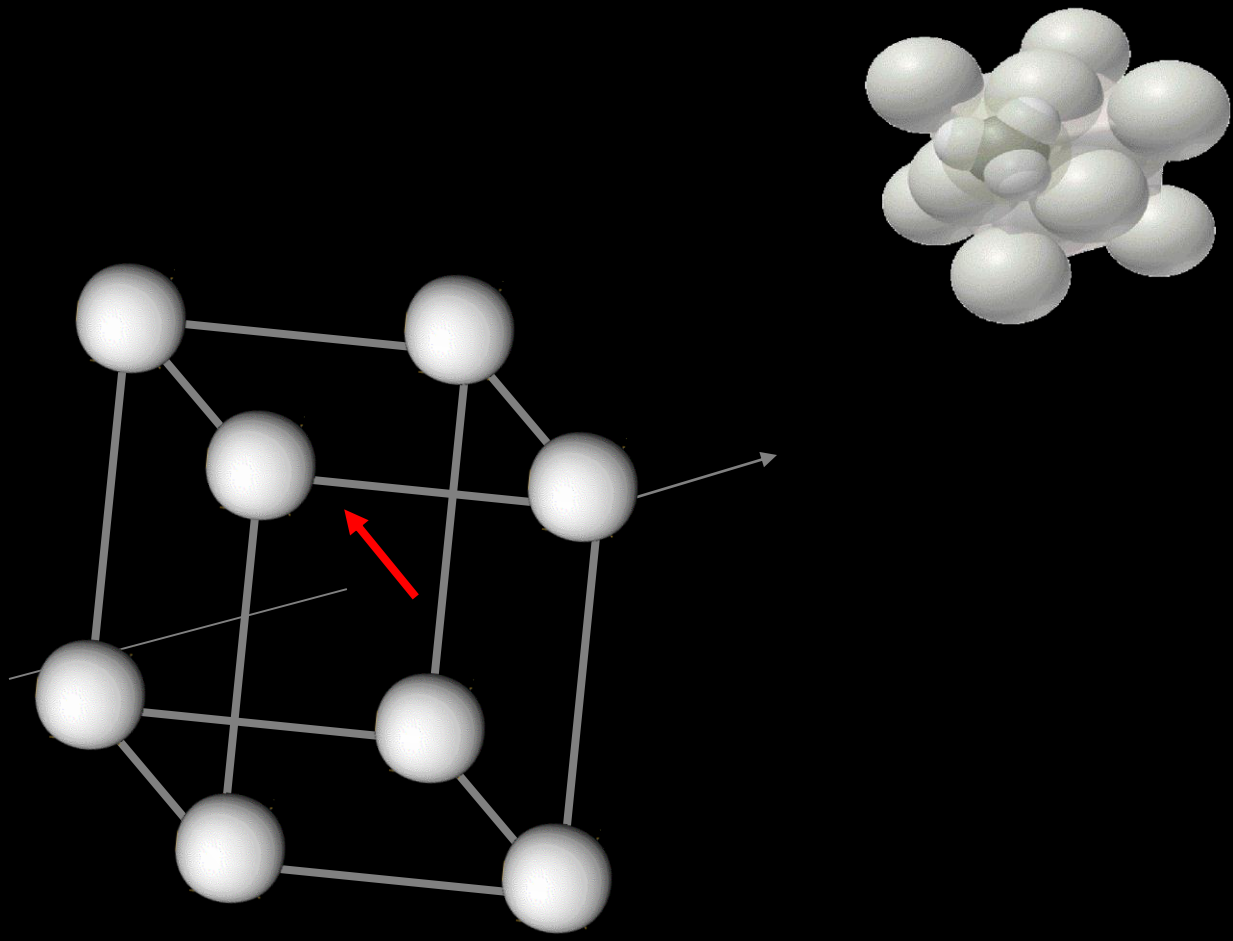


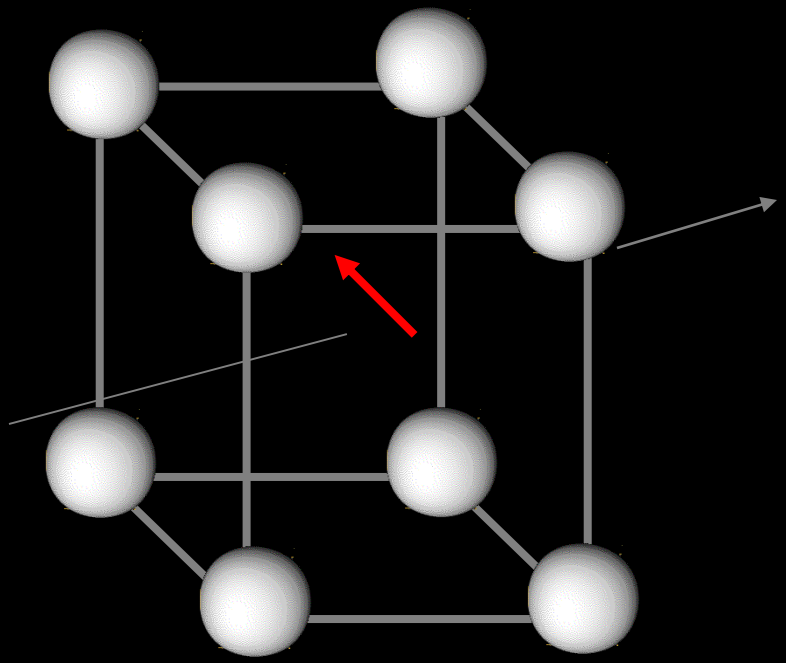


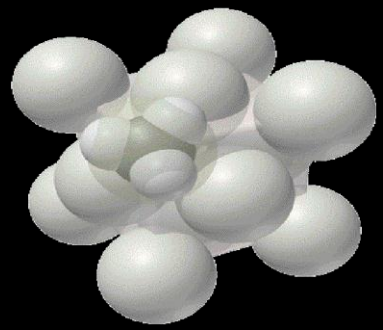






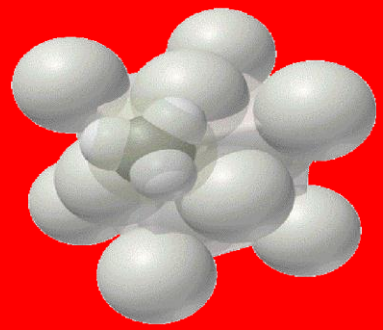


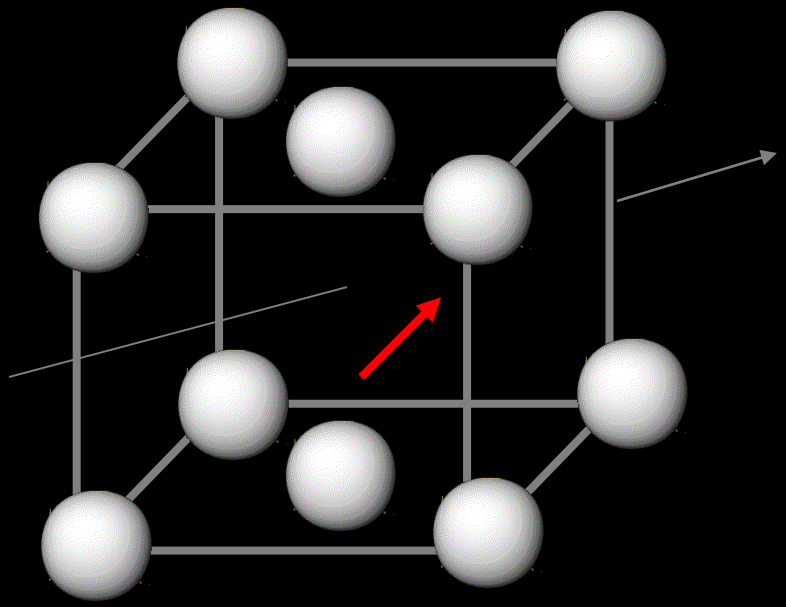


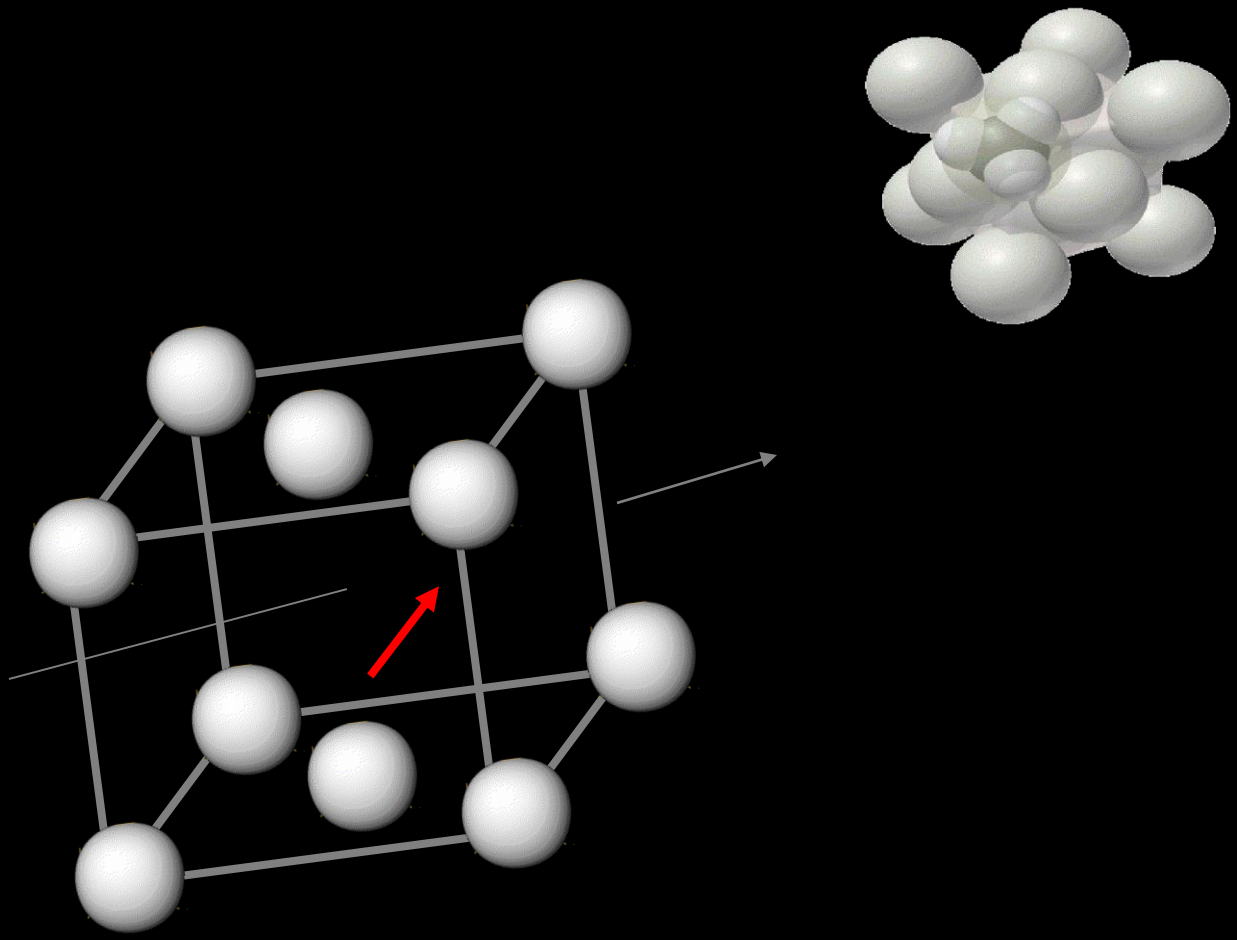


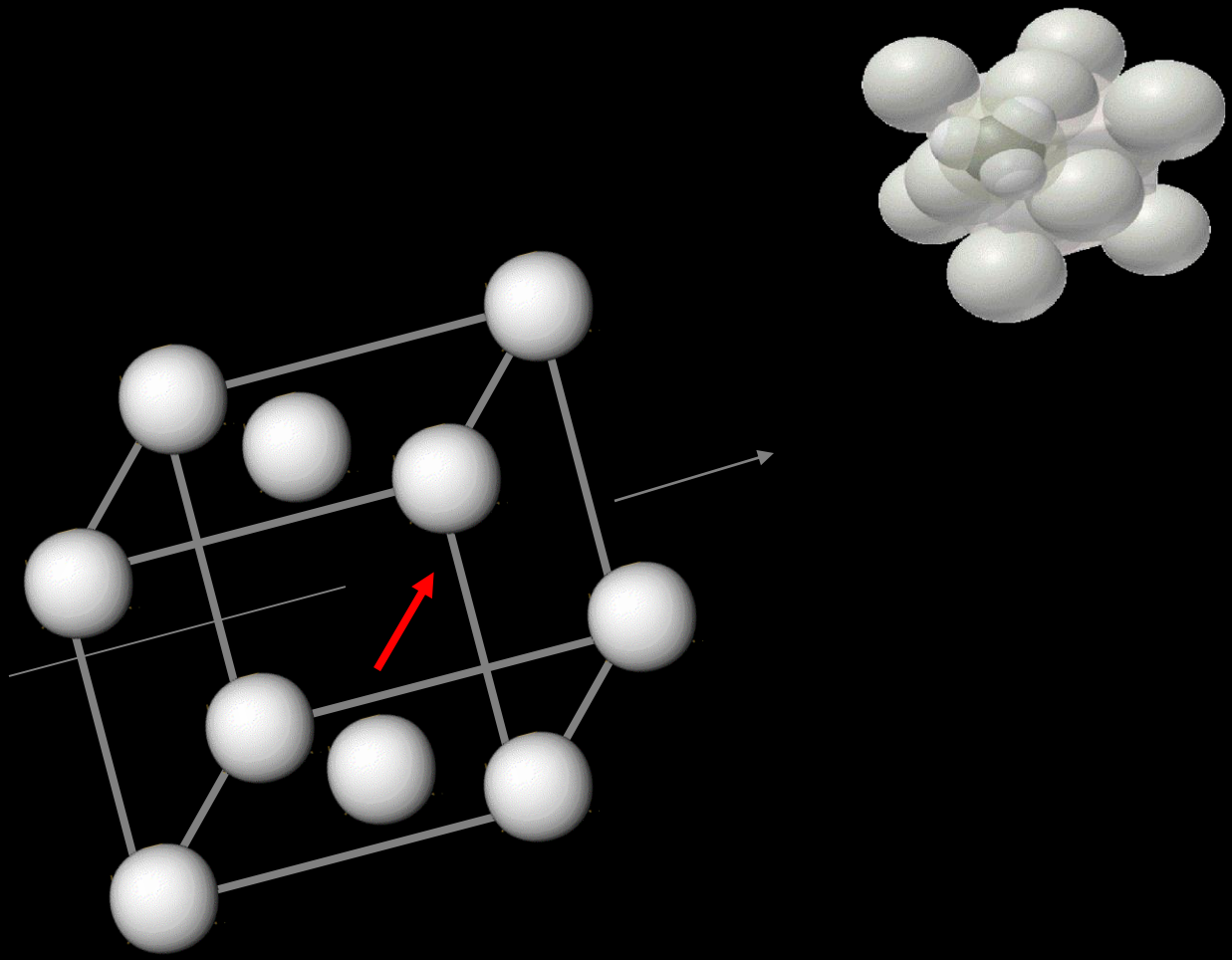
If we do the same with BCC & FCC we will get the same result.

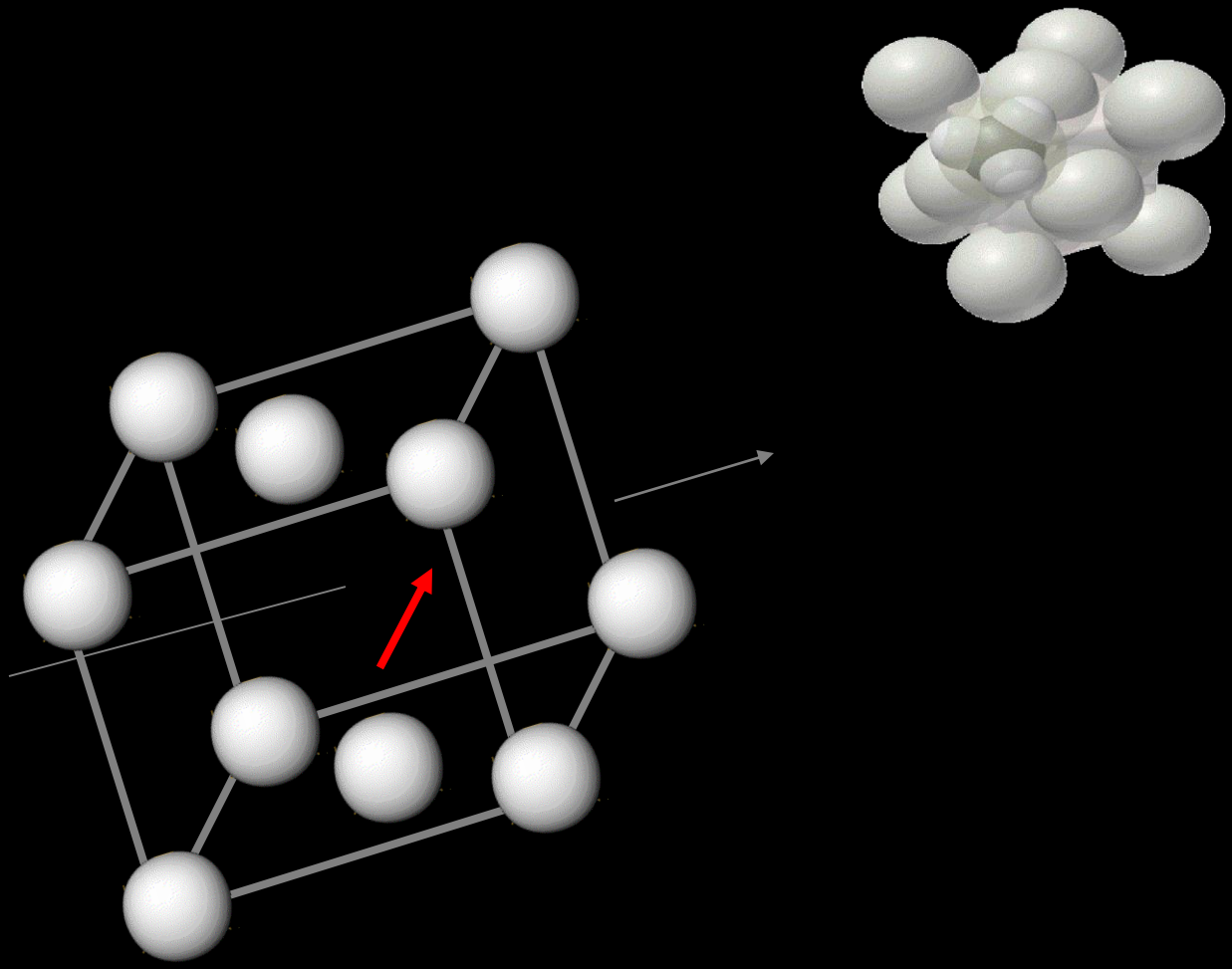
Lets try with End Centered

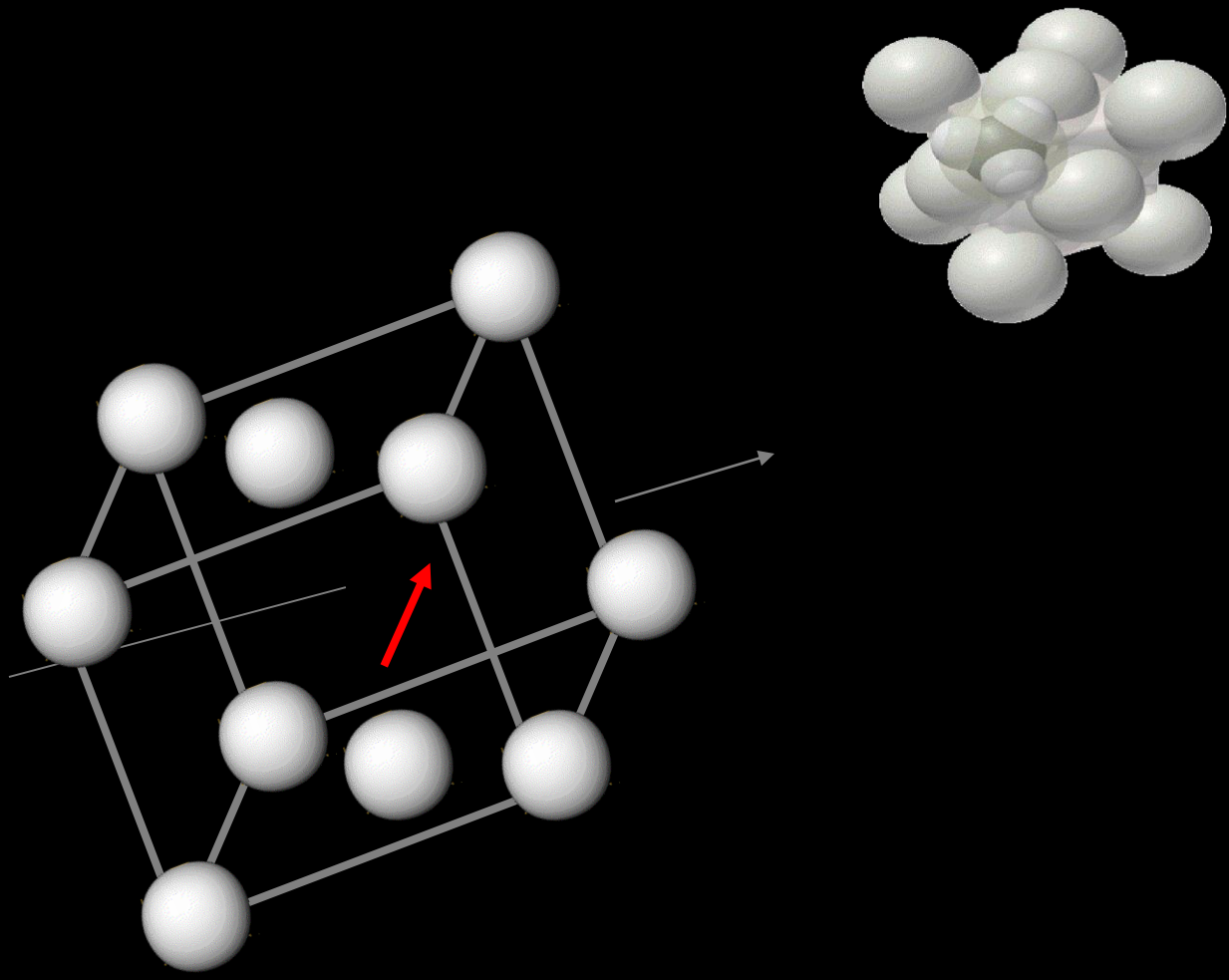


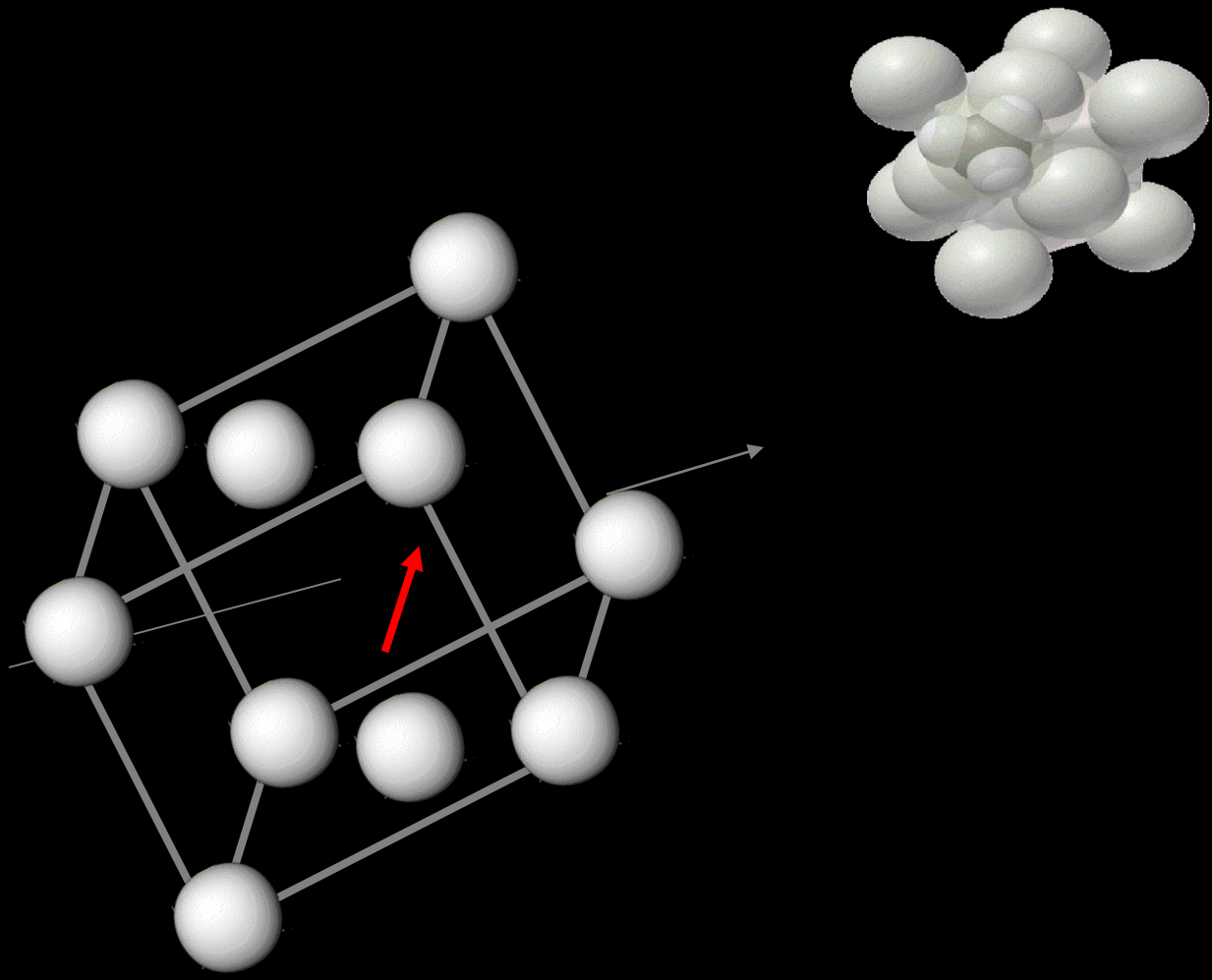


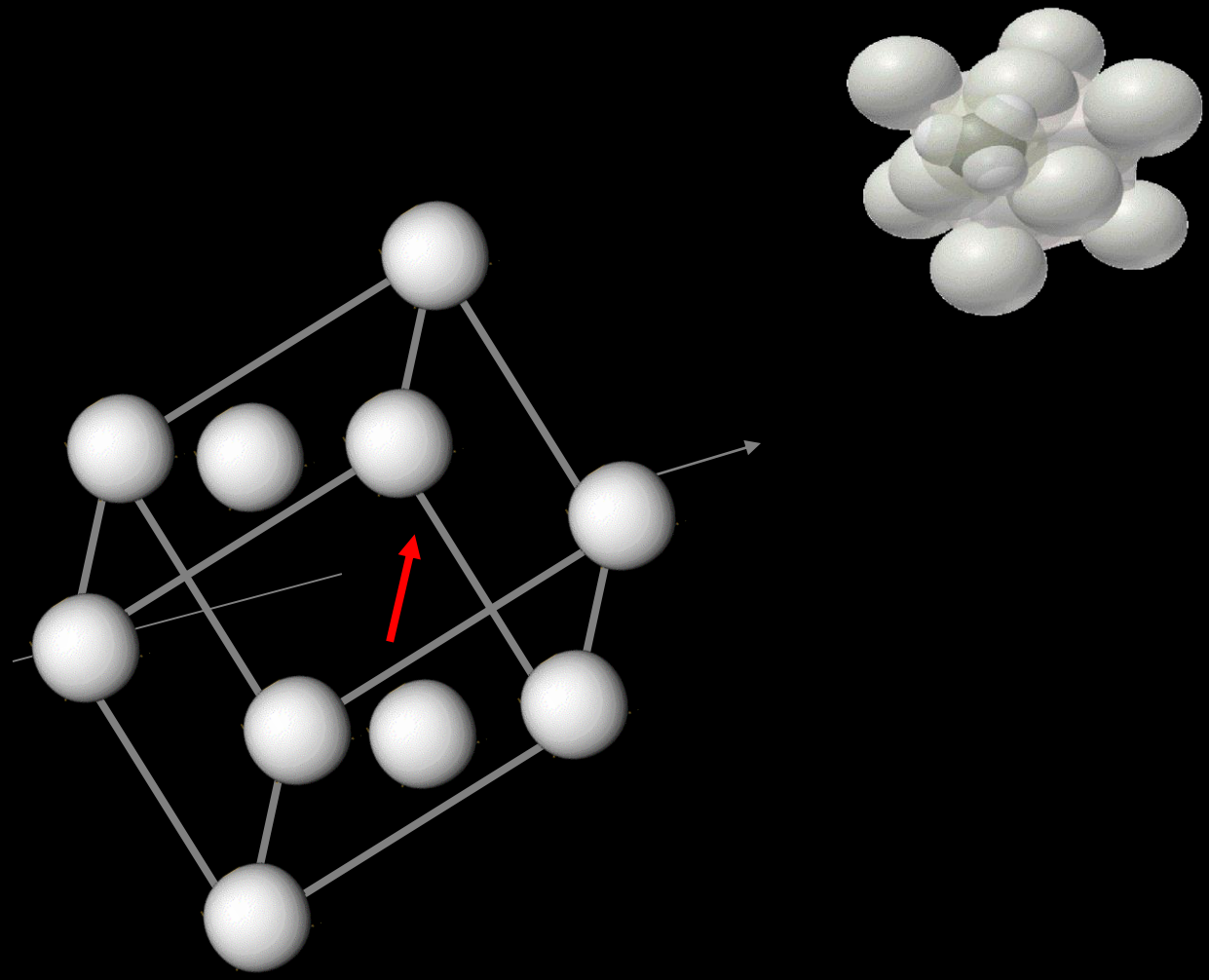


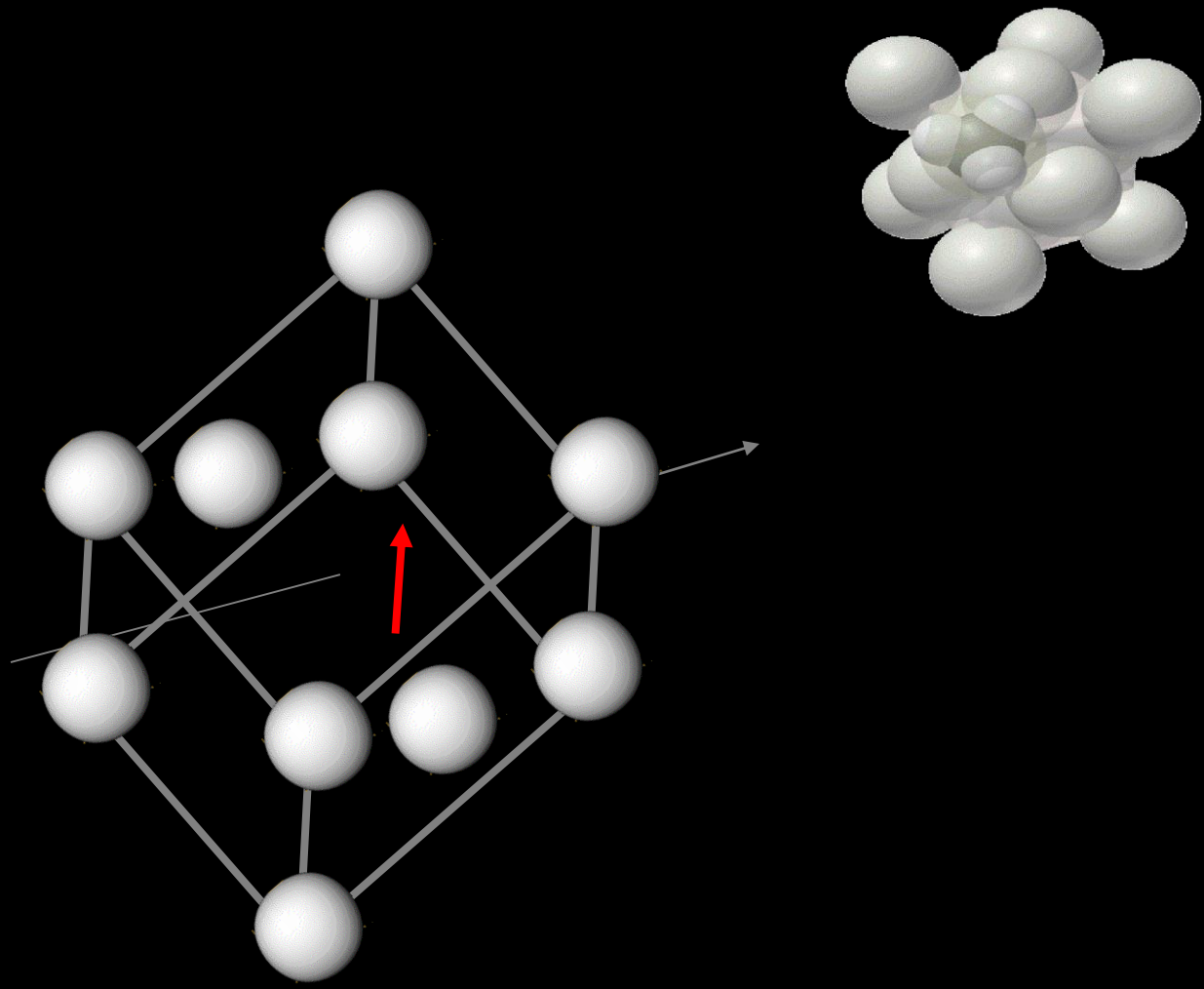


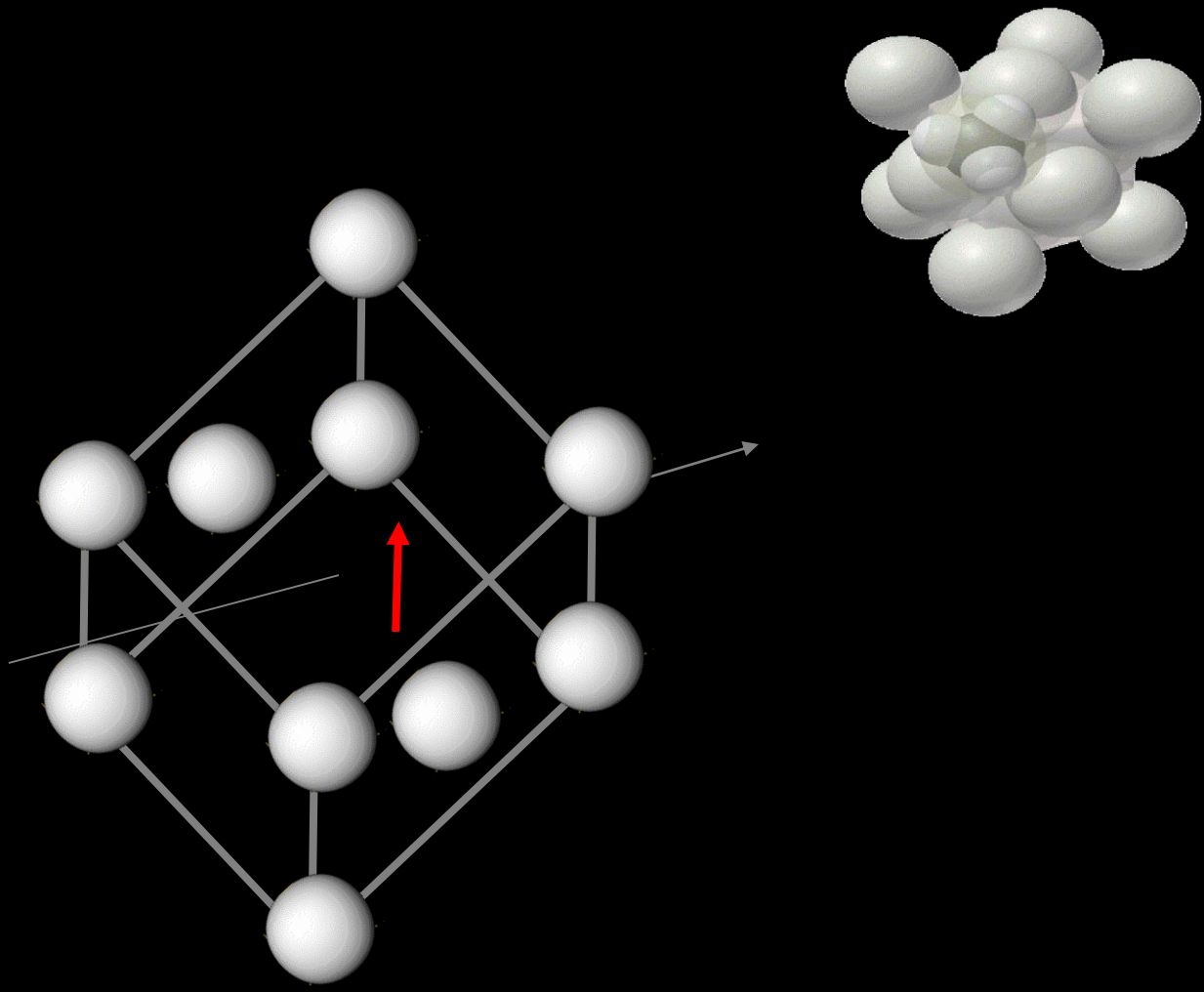


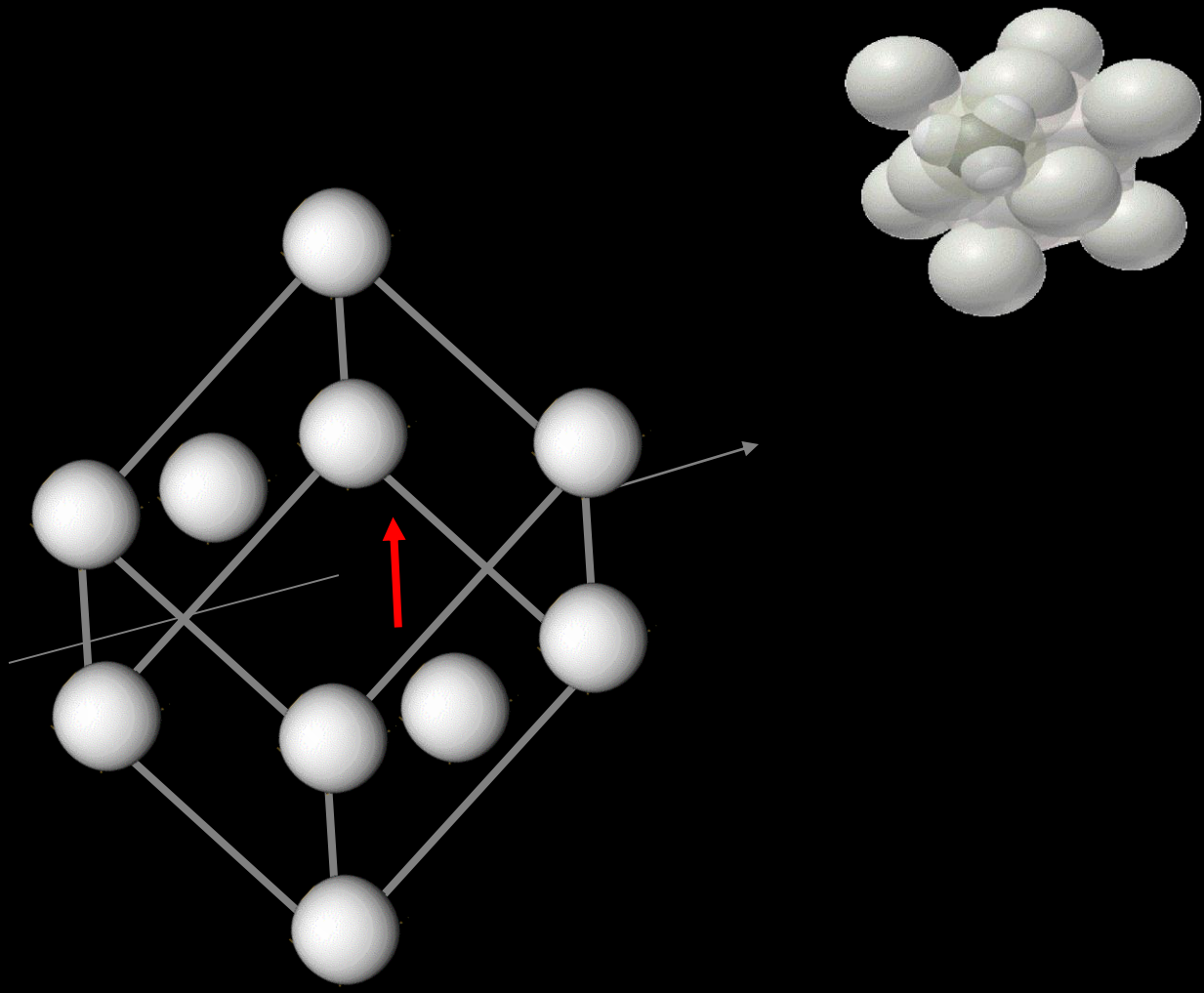


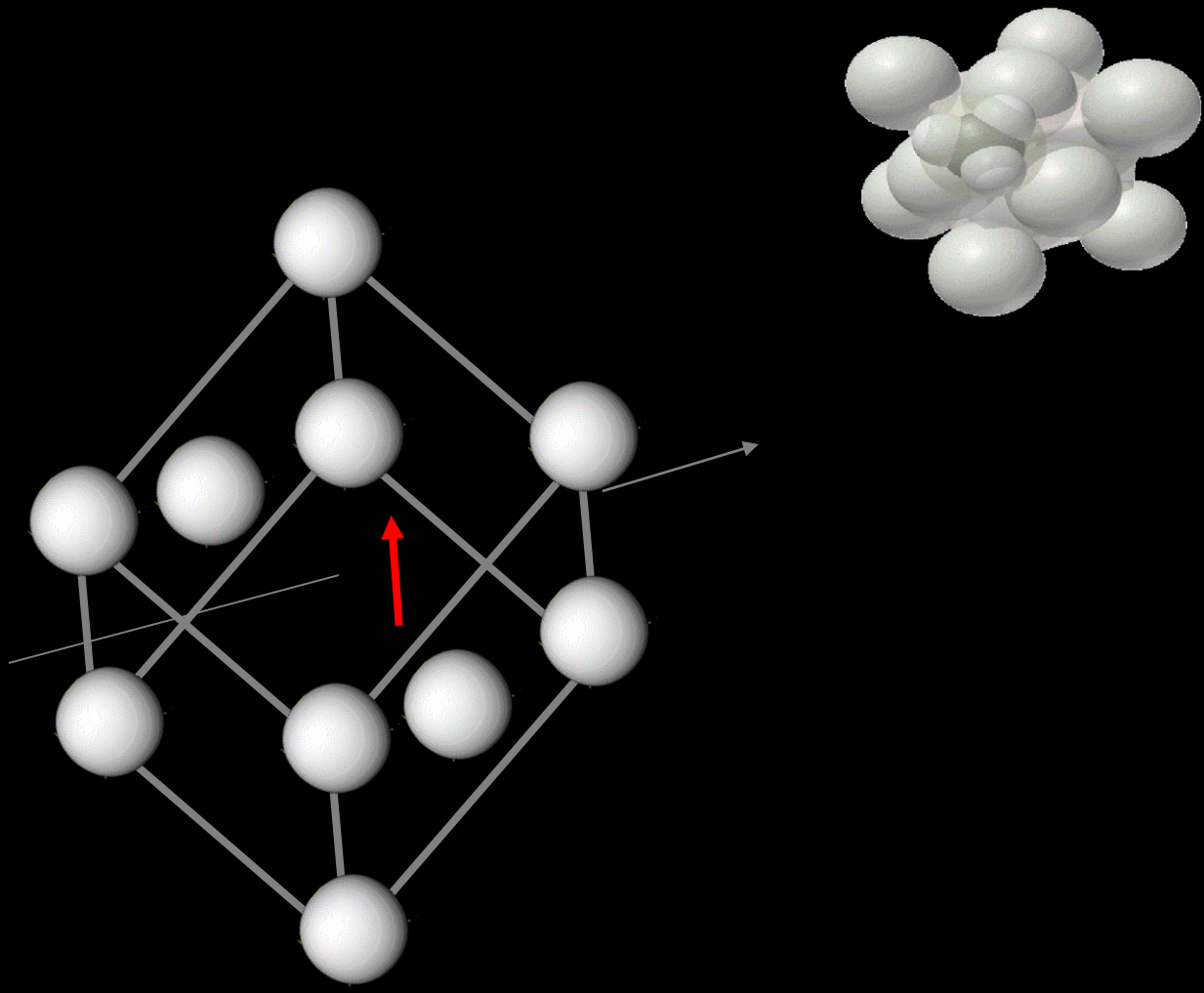


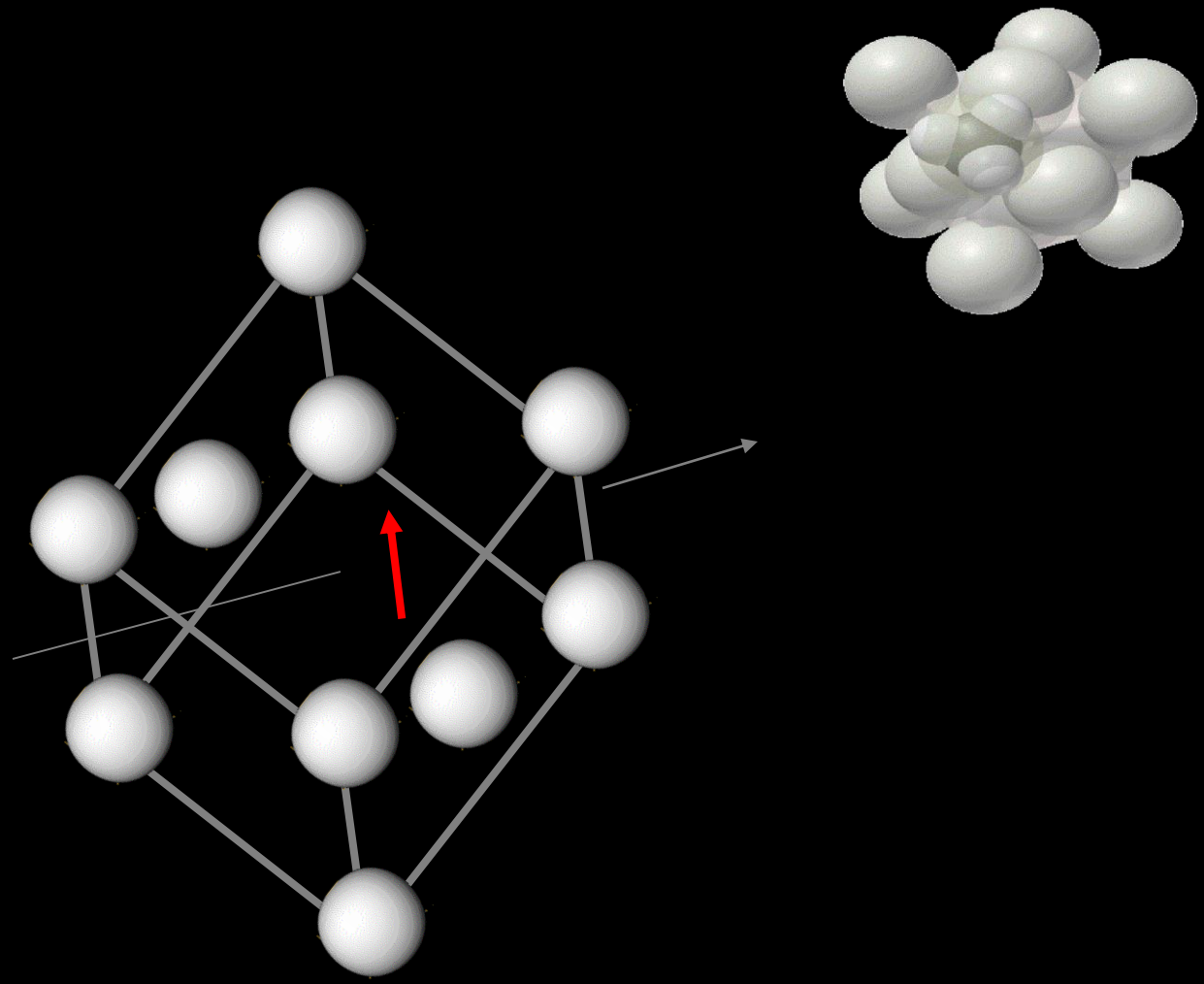


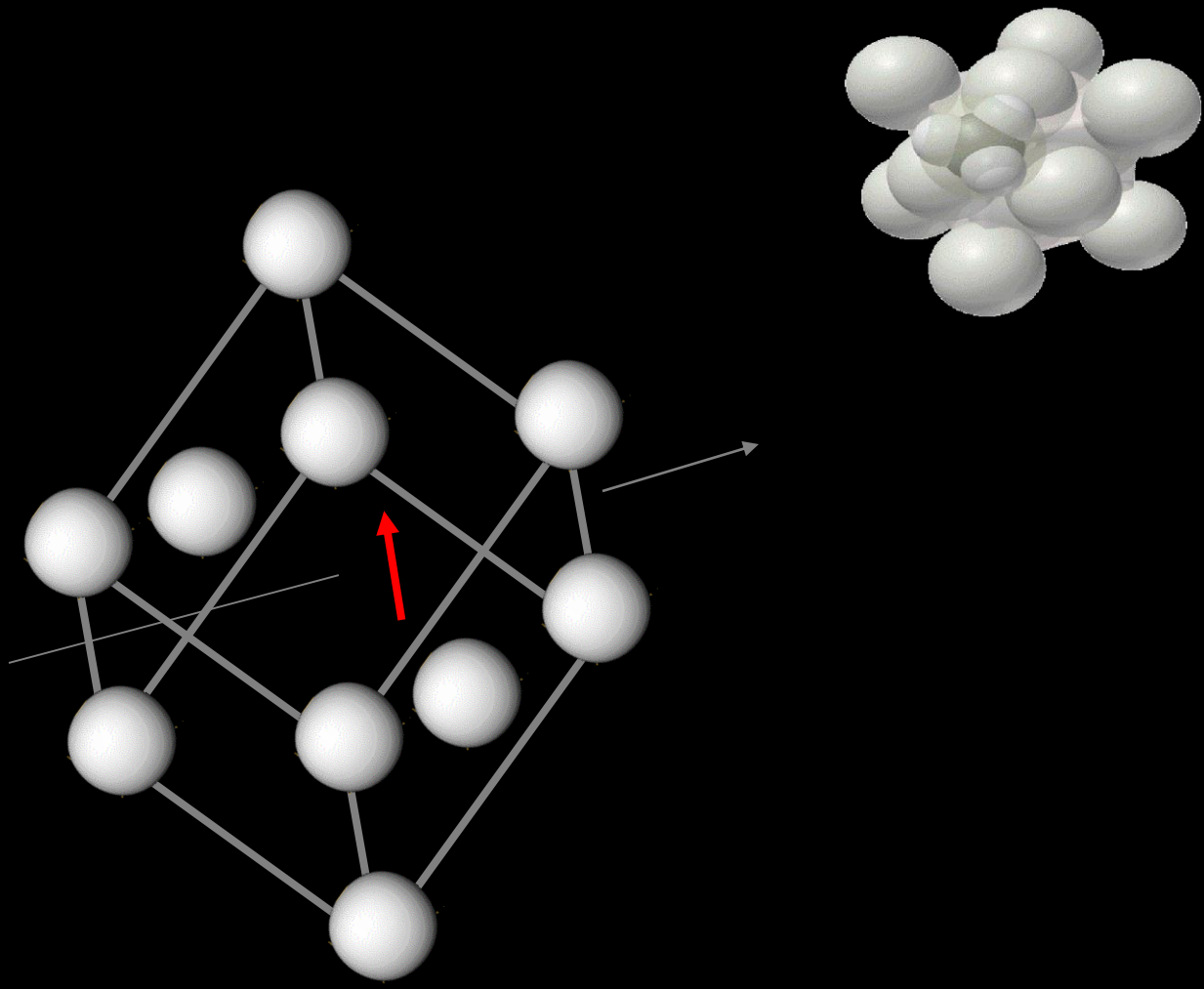


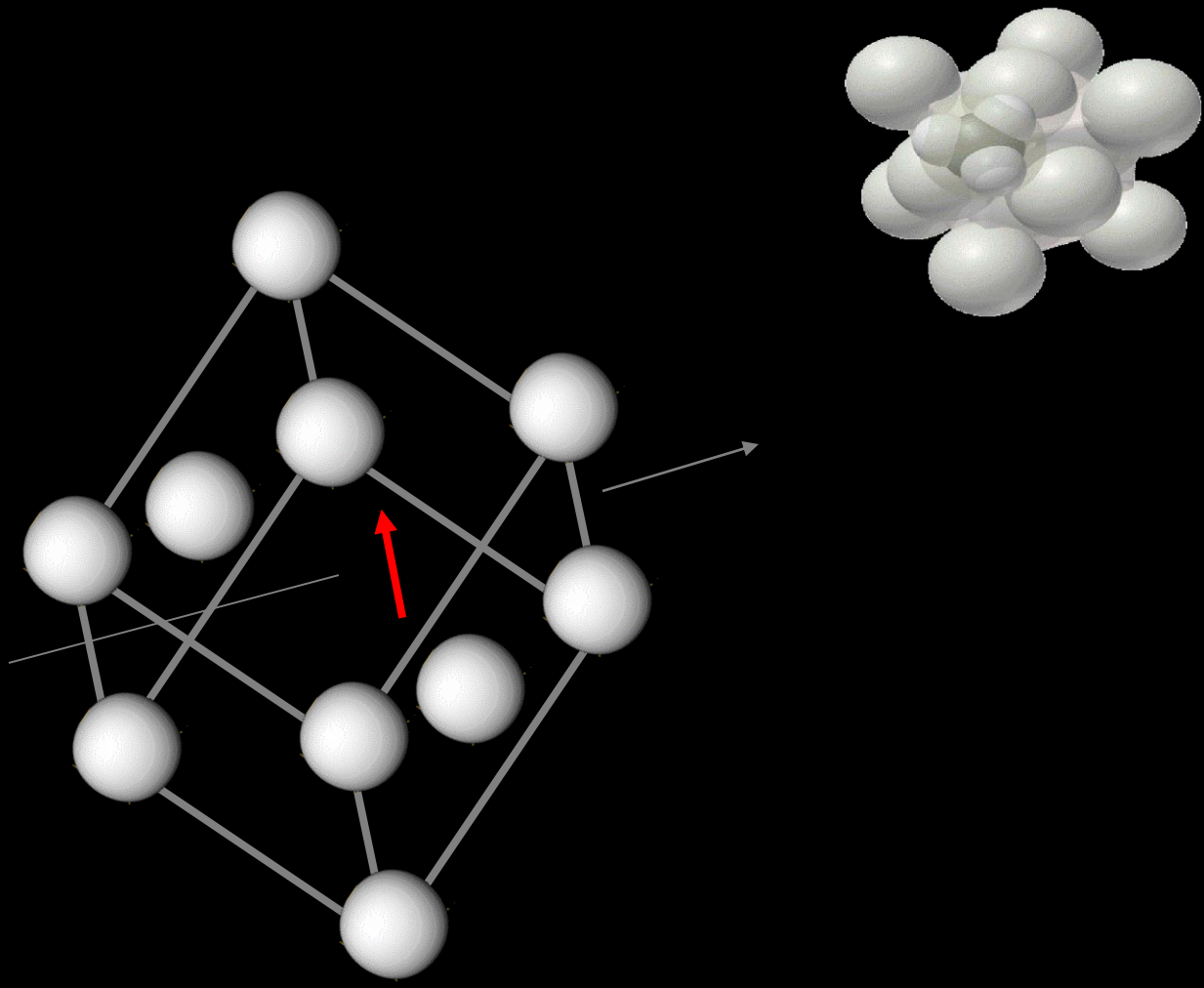


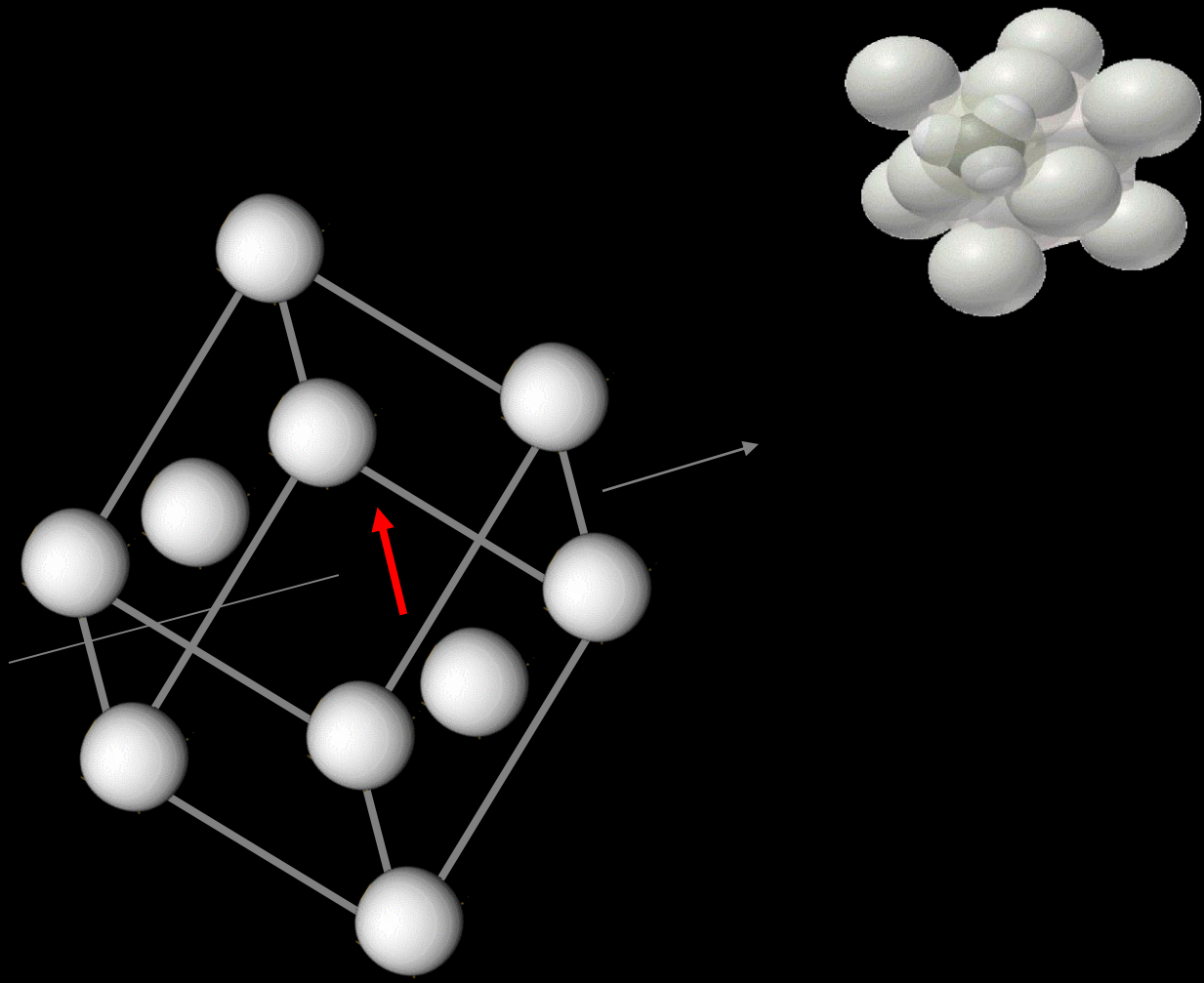


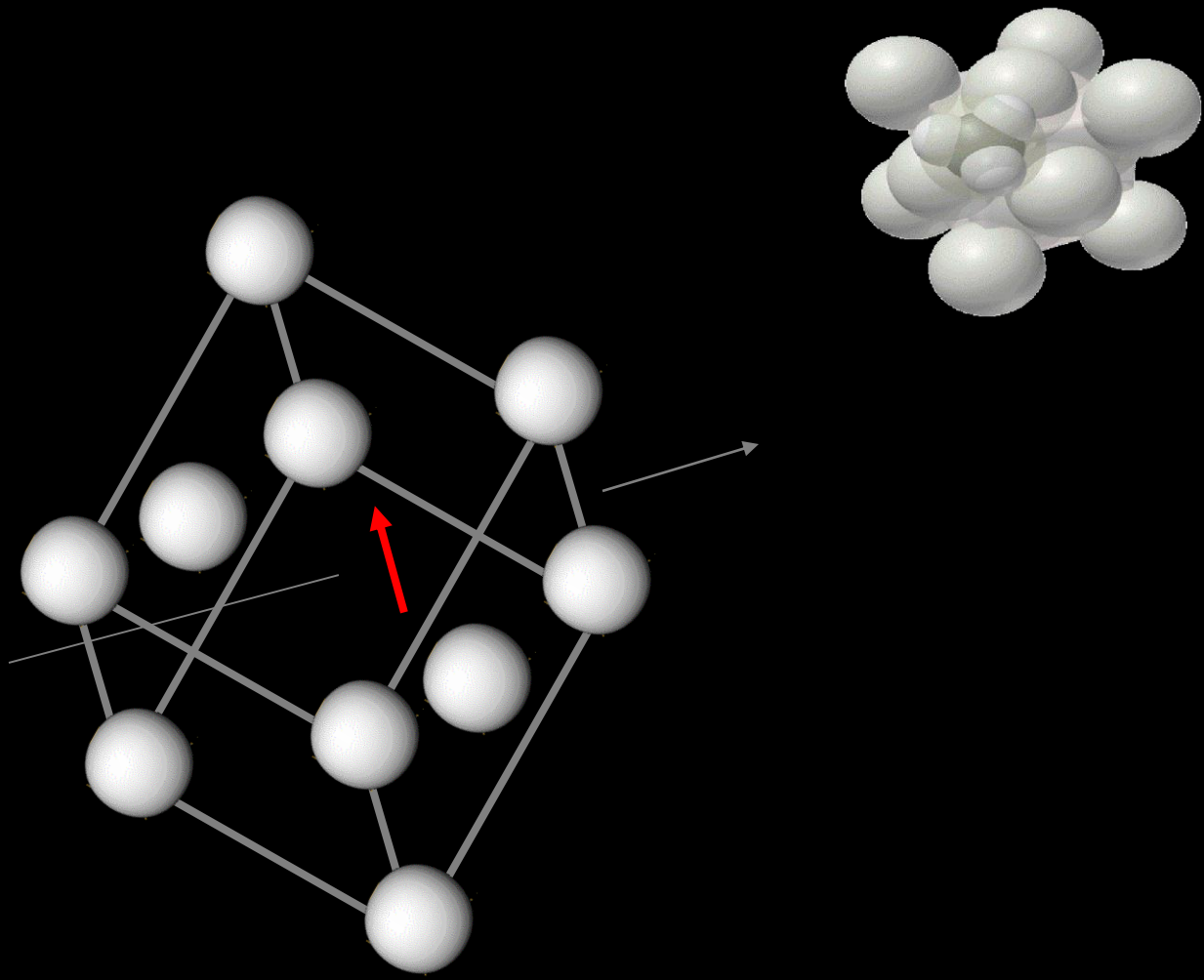


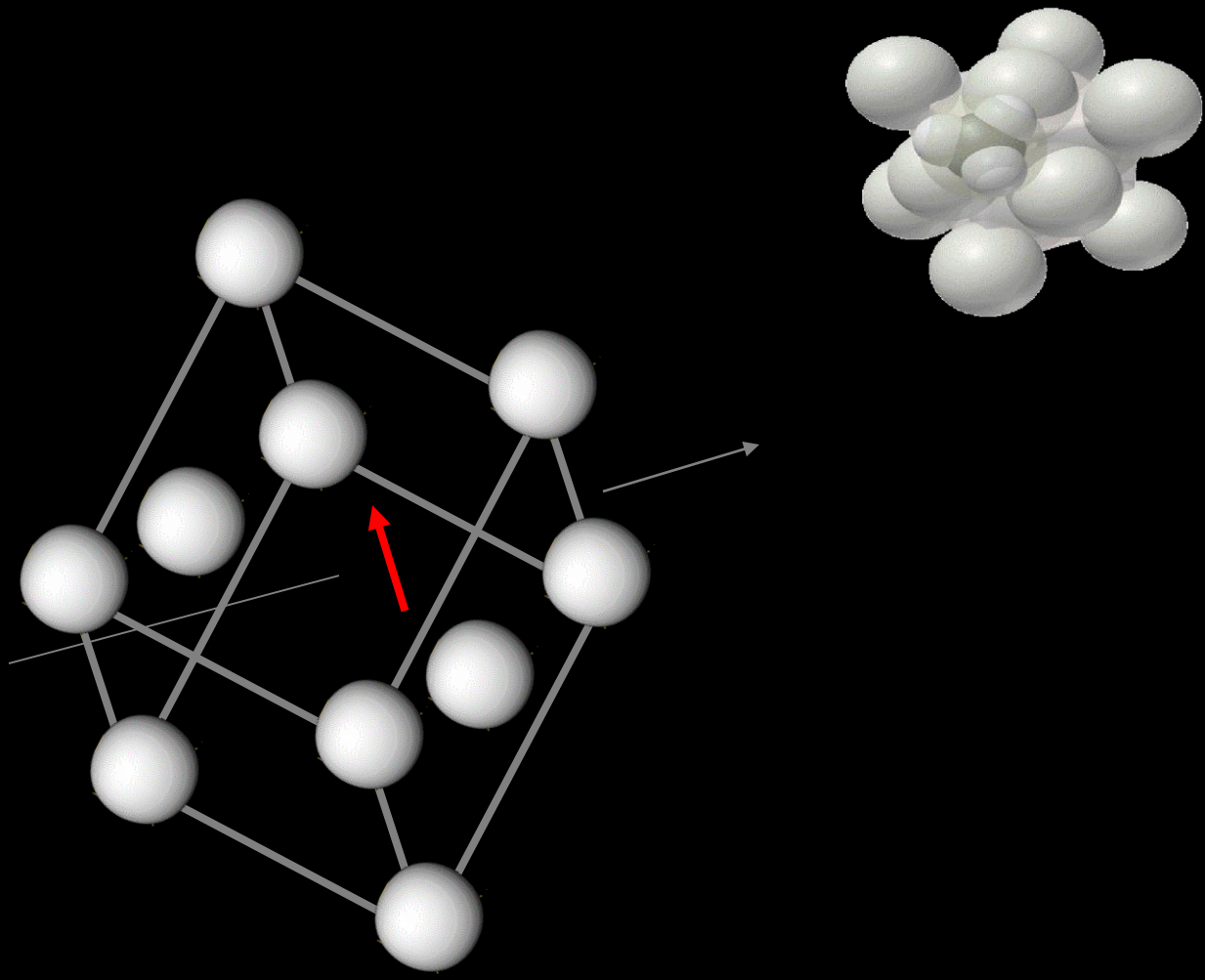


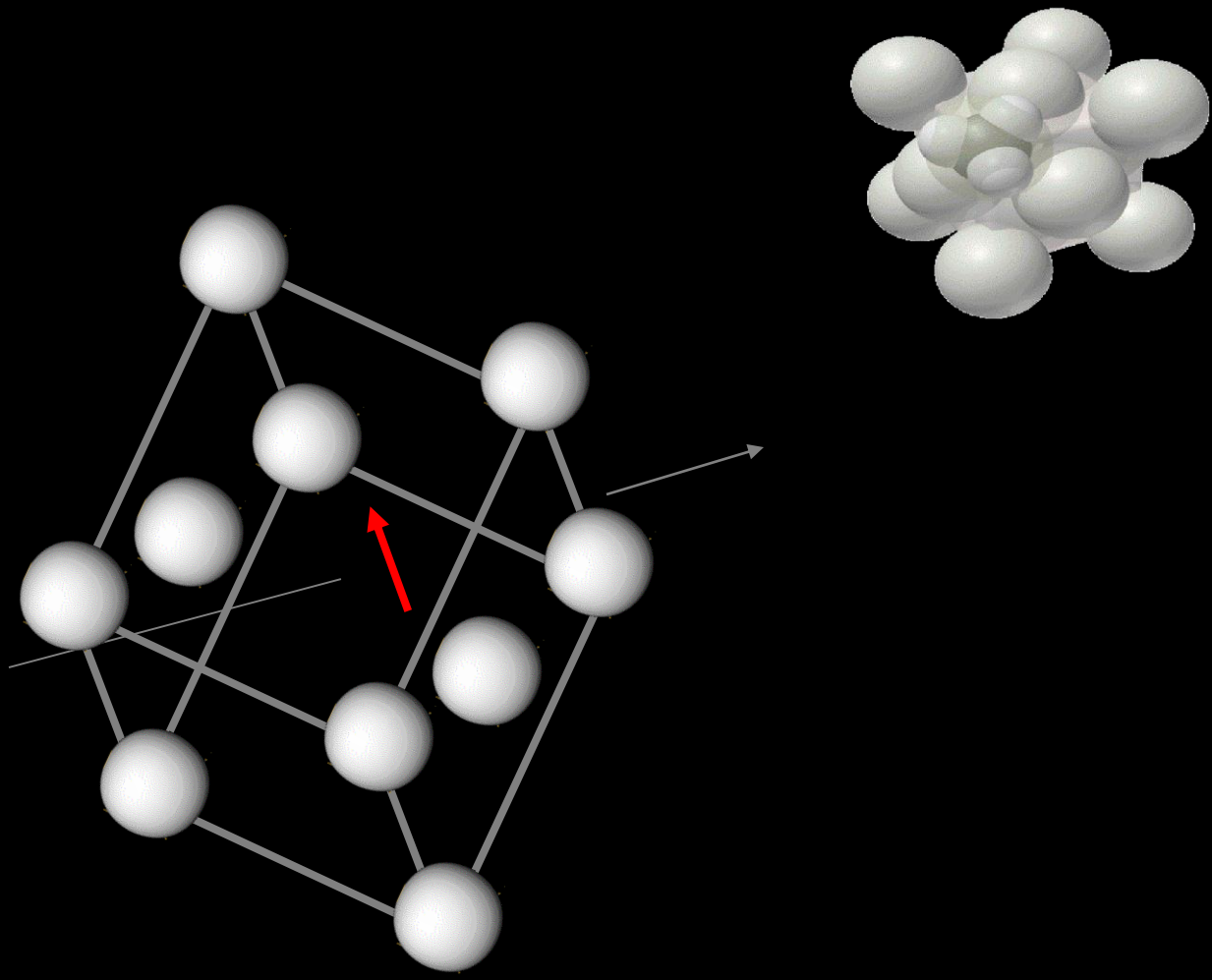


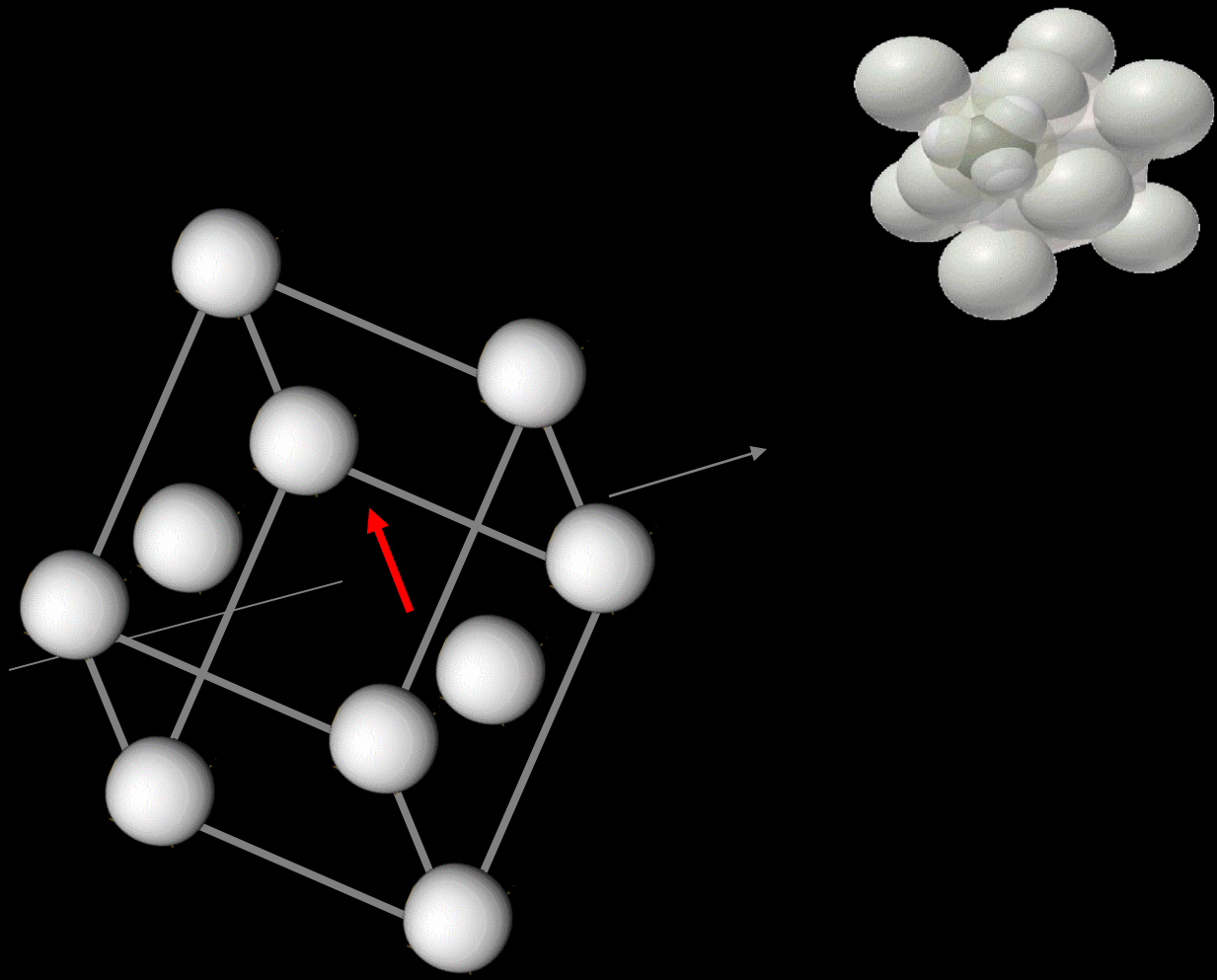


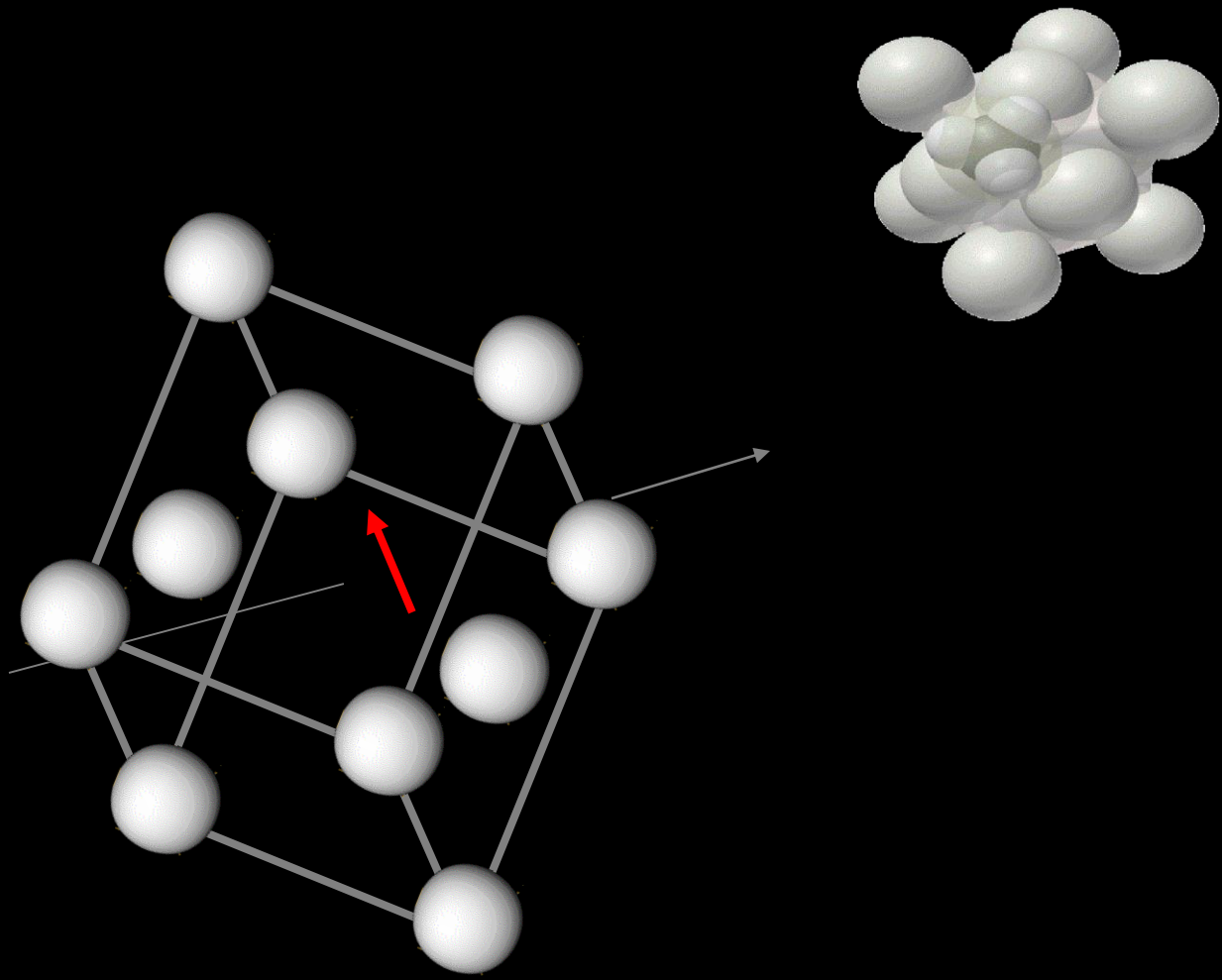


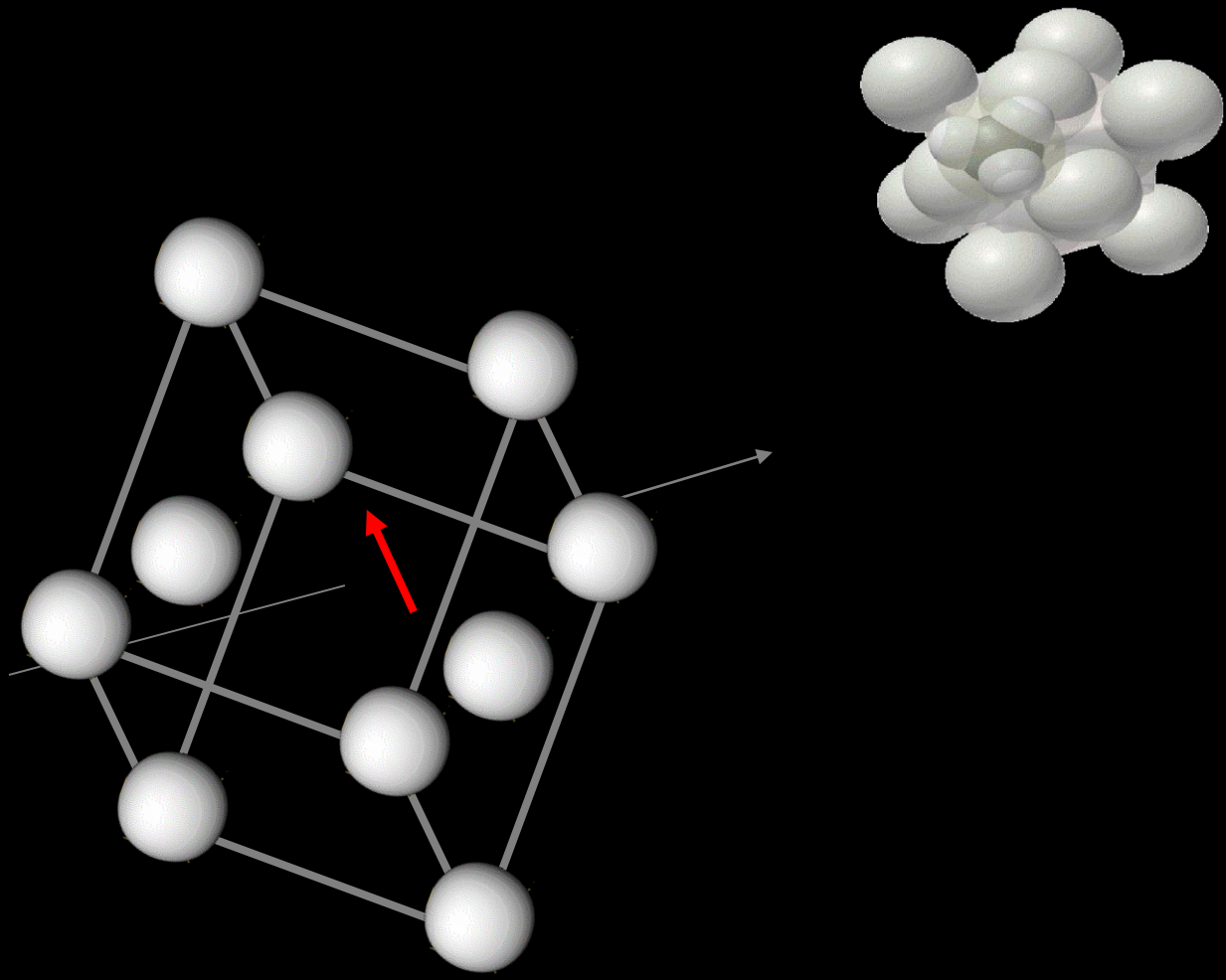


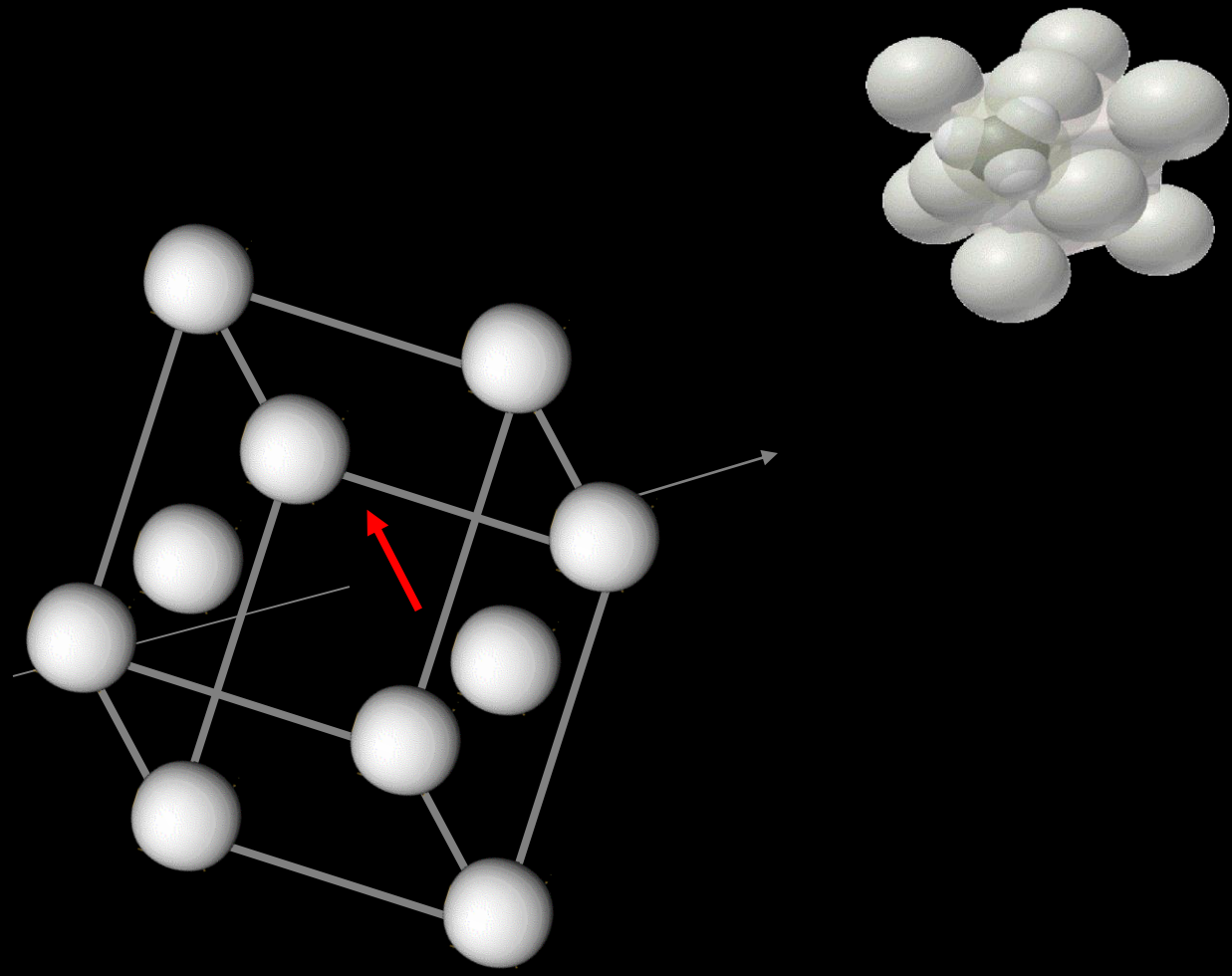


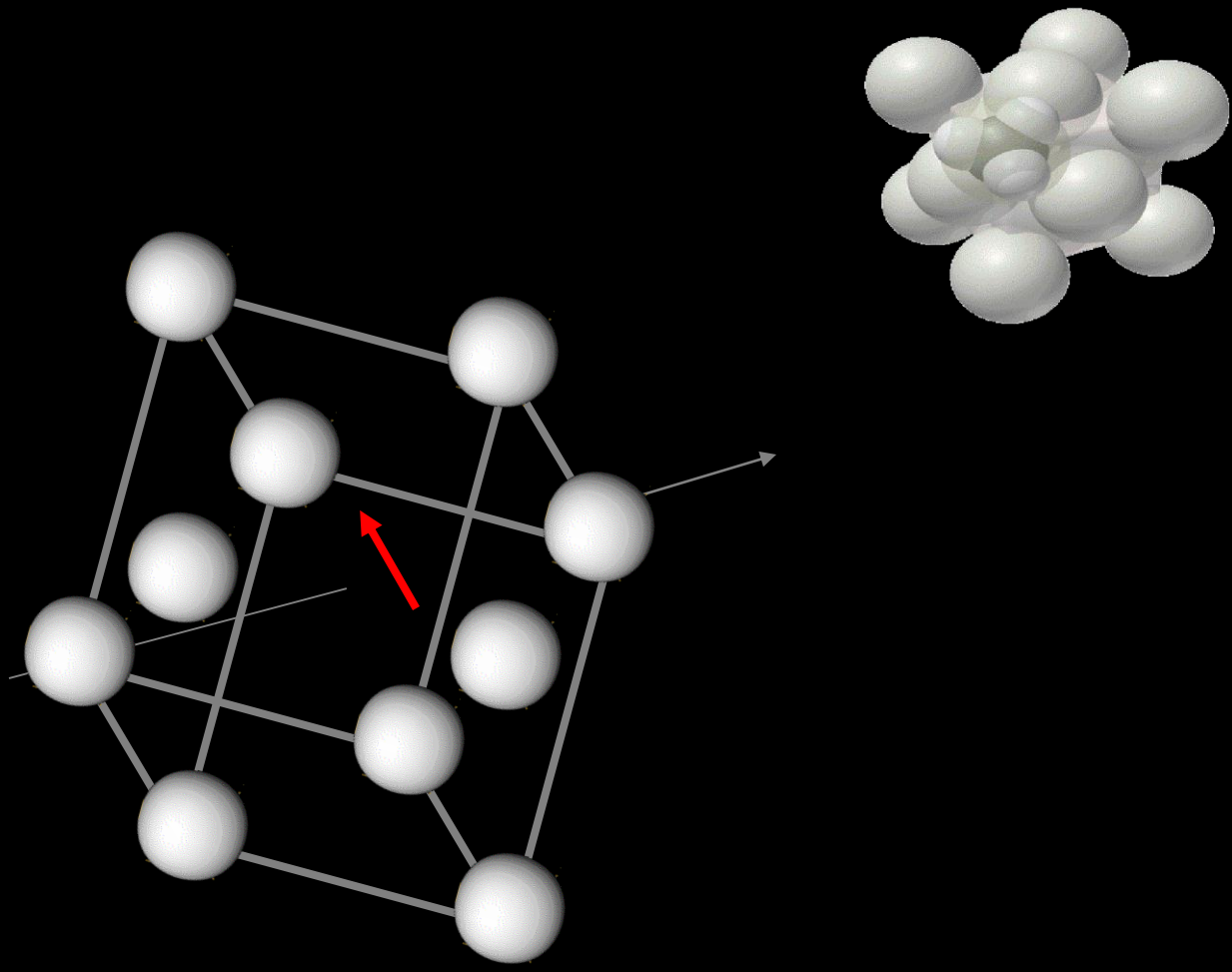


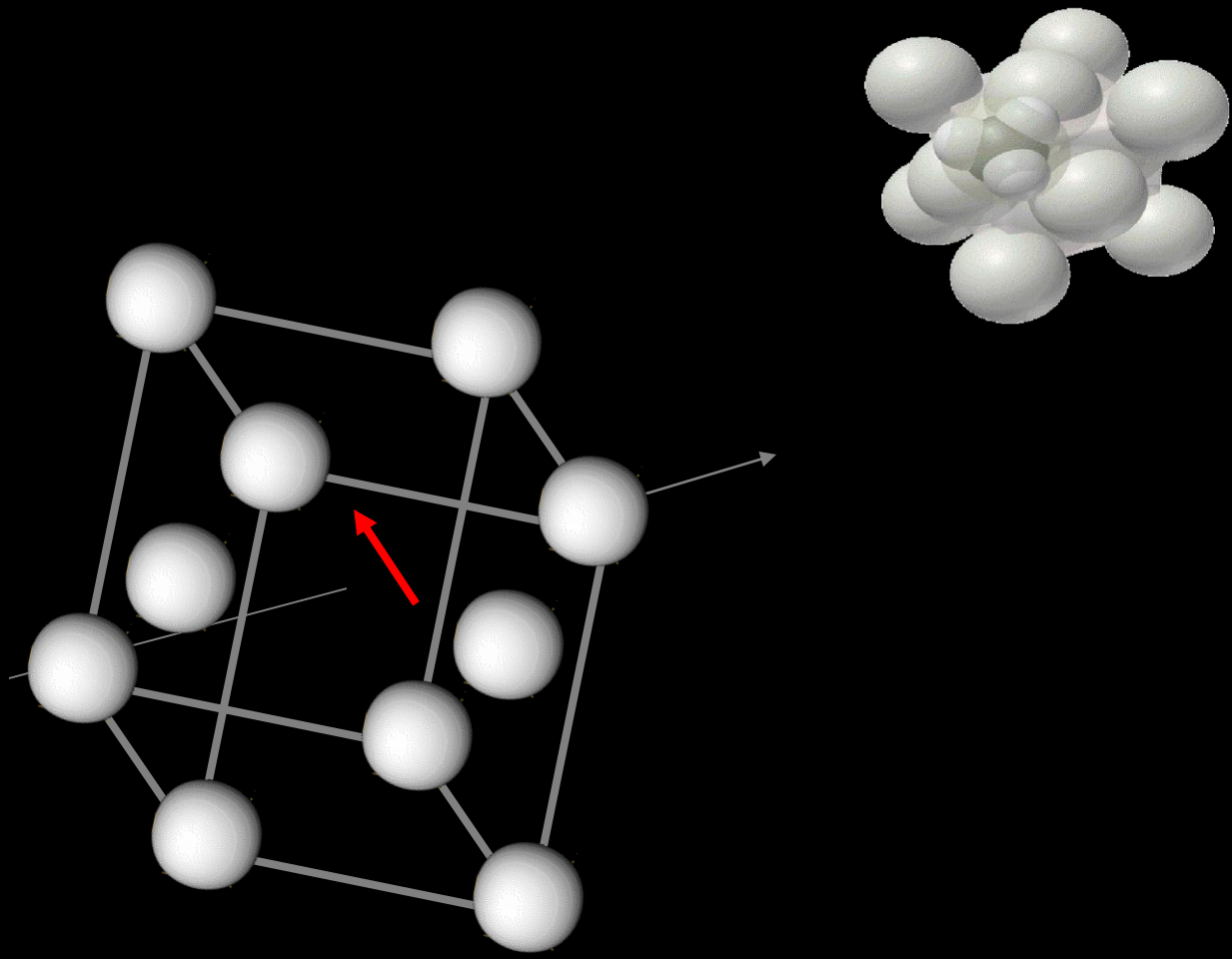


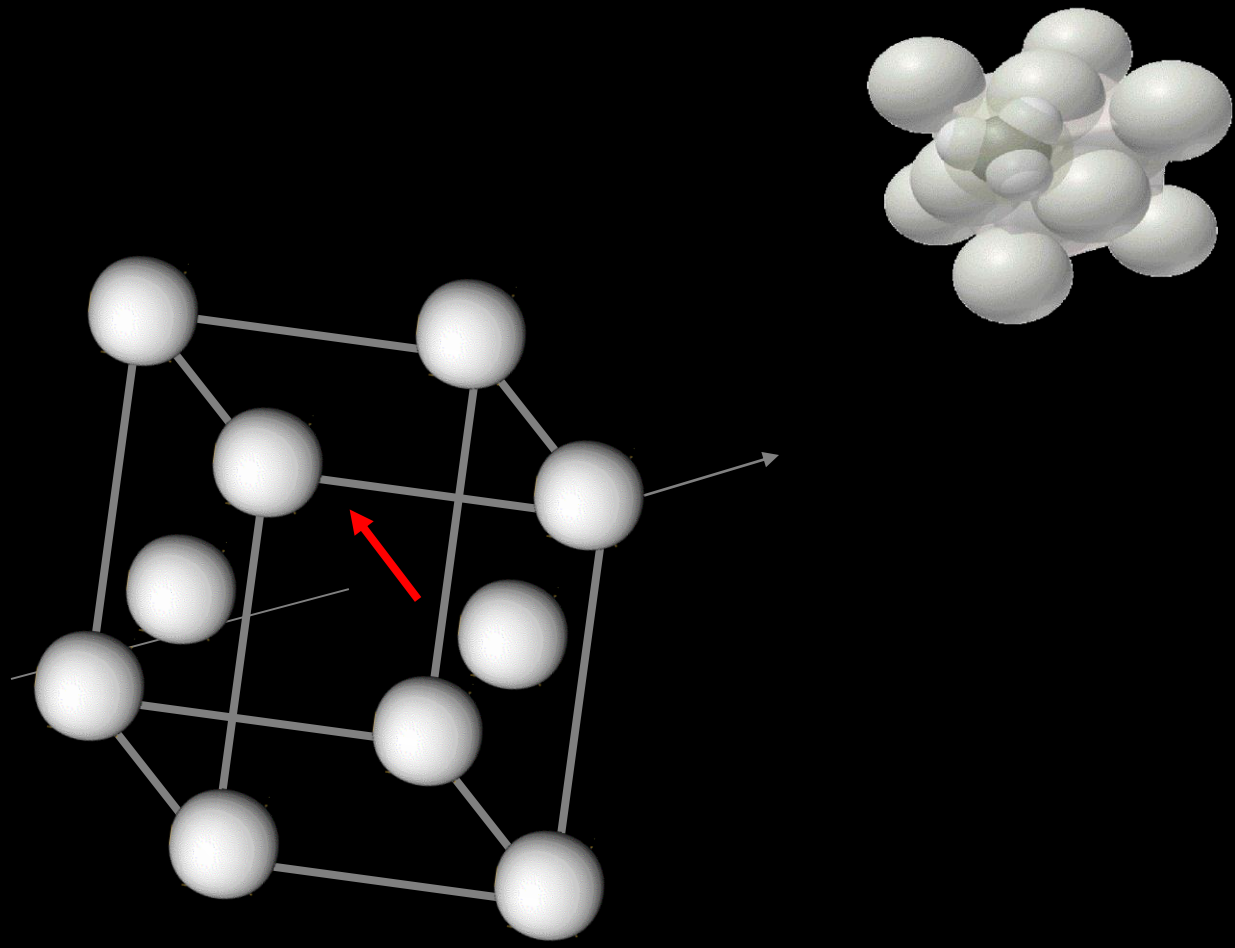


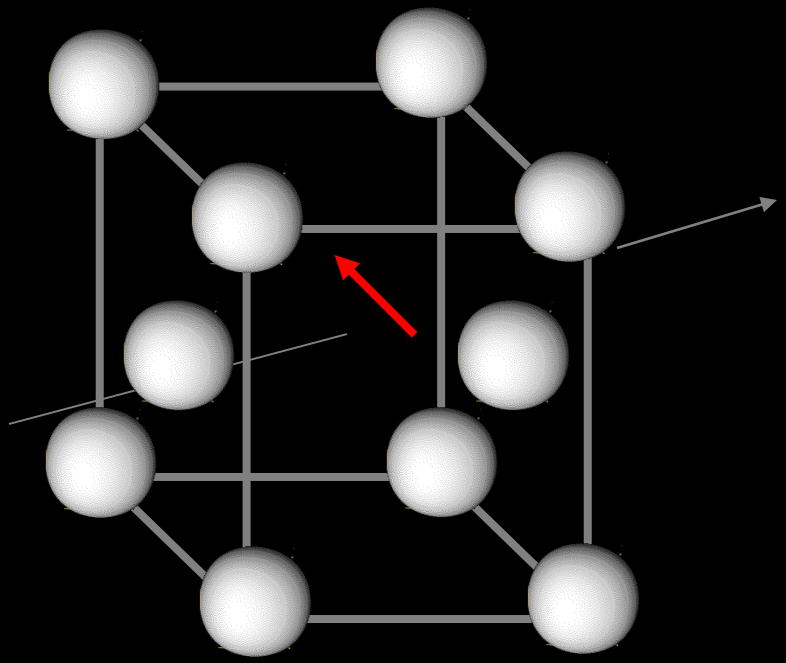


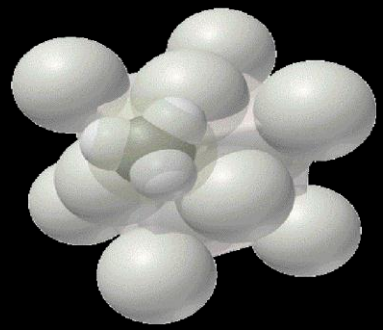




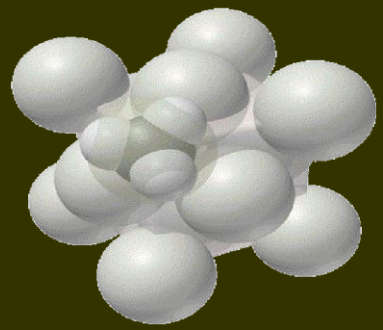




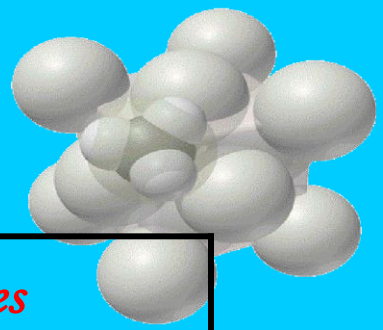




Like this 13 other arrangements in various shapes were rejected.

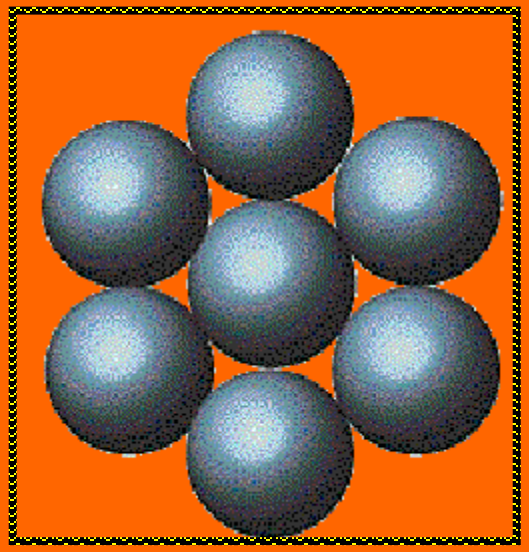


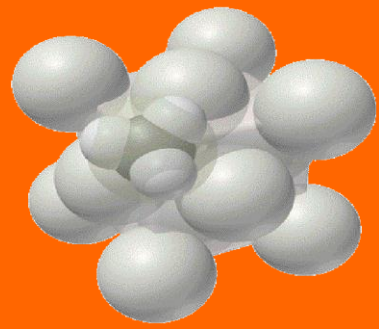
We are left with only 14 unit cells



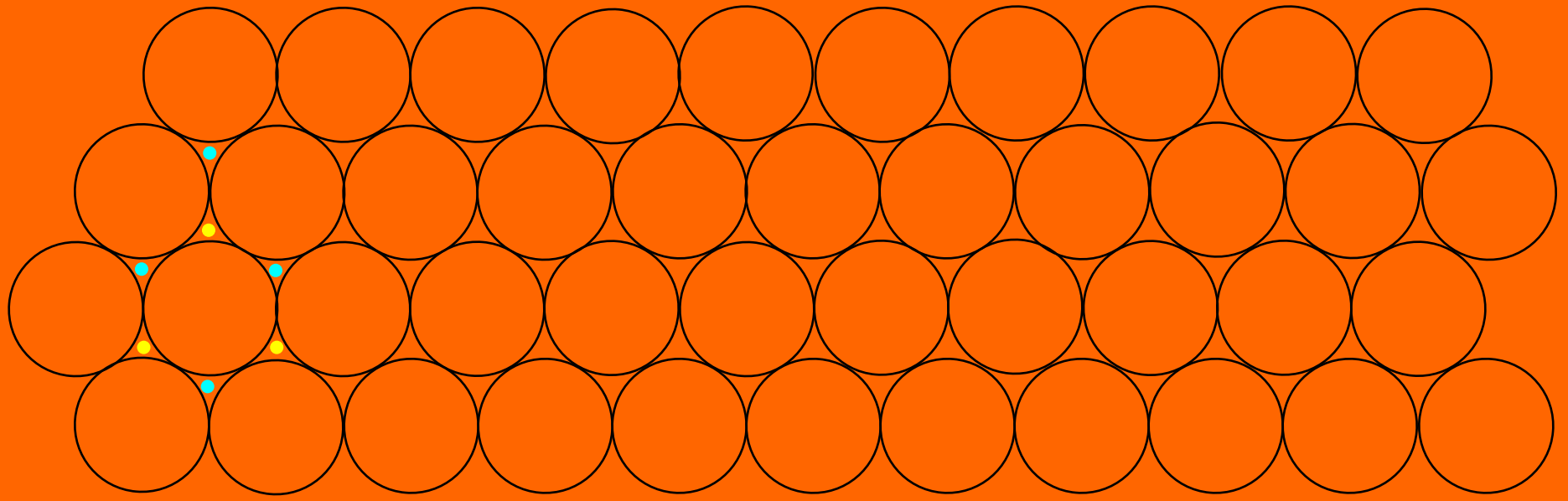
Crystal Systems	Bravais Lattices
Cubic	Primitive, FCC, BCC
Orthorhombic	Primitive, FC, BC, EC
Rhombohedral	Primitive
Tetragonal	Primitive, BC
Triclinic	Primitive
Hexagonal	Primitive
Monoclinic	Primitive, EC

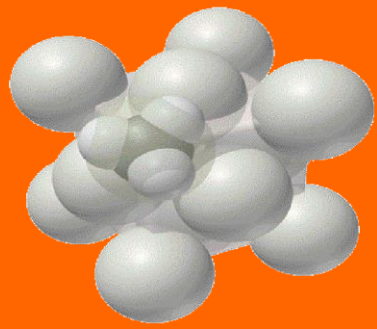
Layer arrangement view



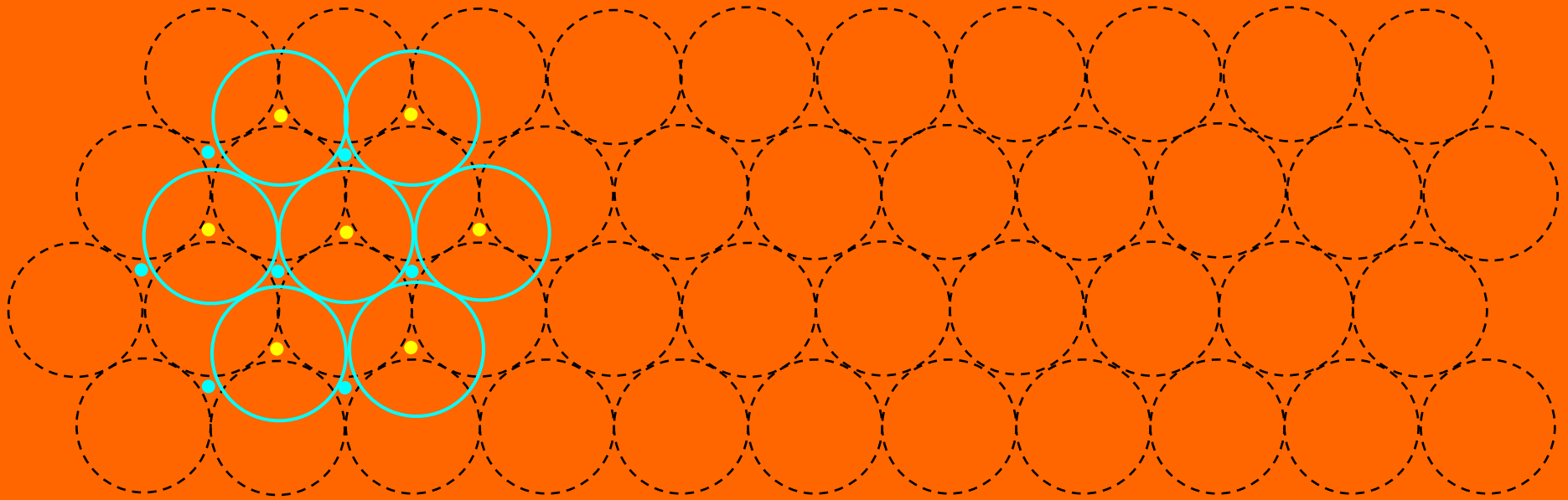


Layer A



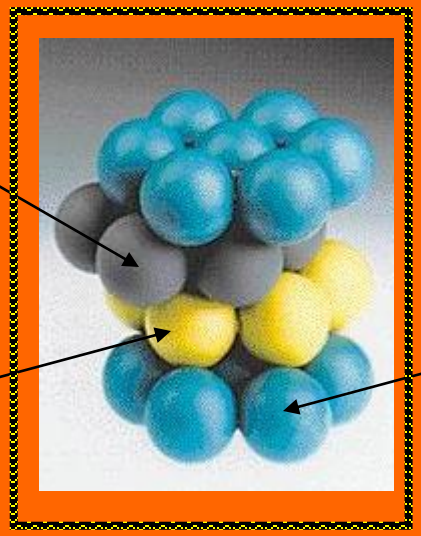


Layer B



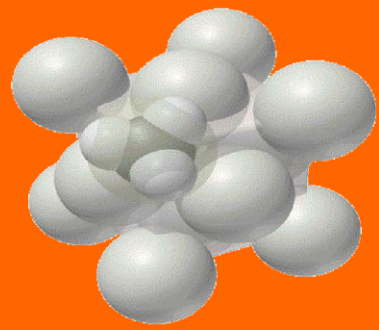
Layer C

Cubic Close Packing (CCP)

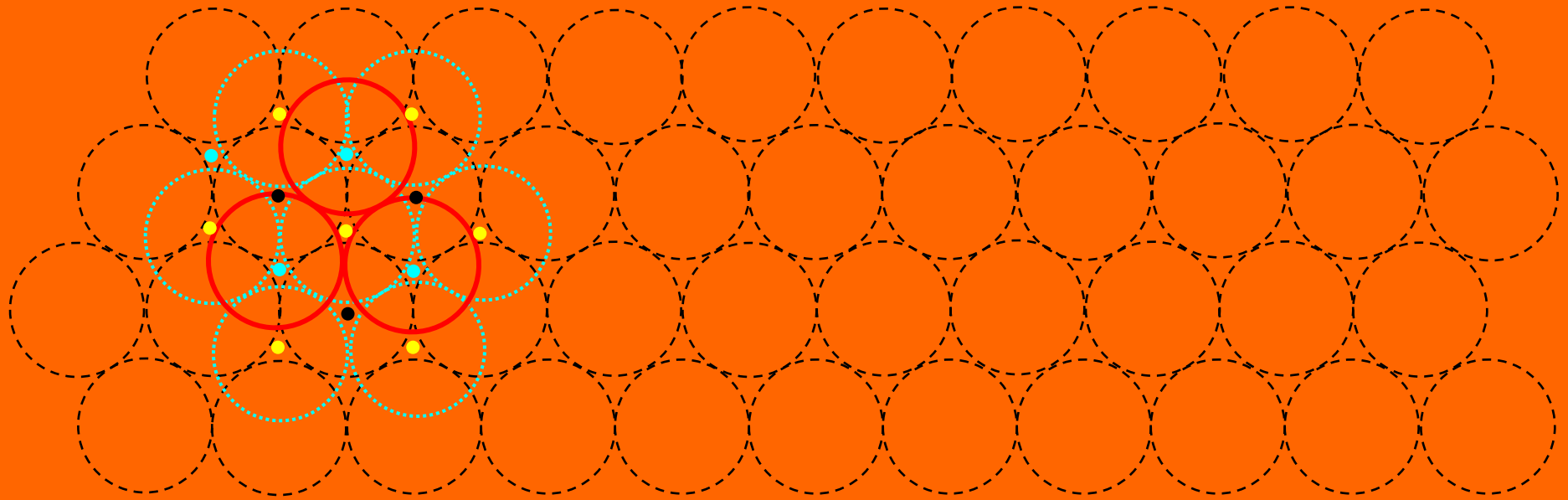


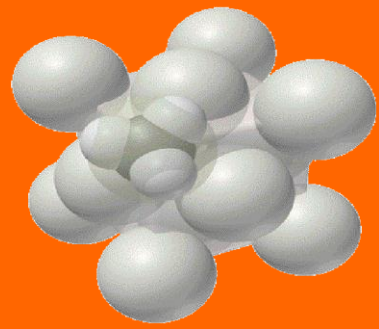
Layer A

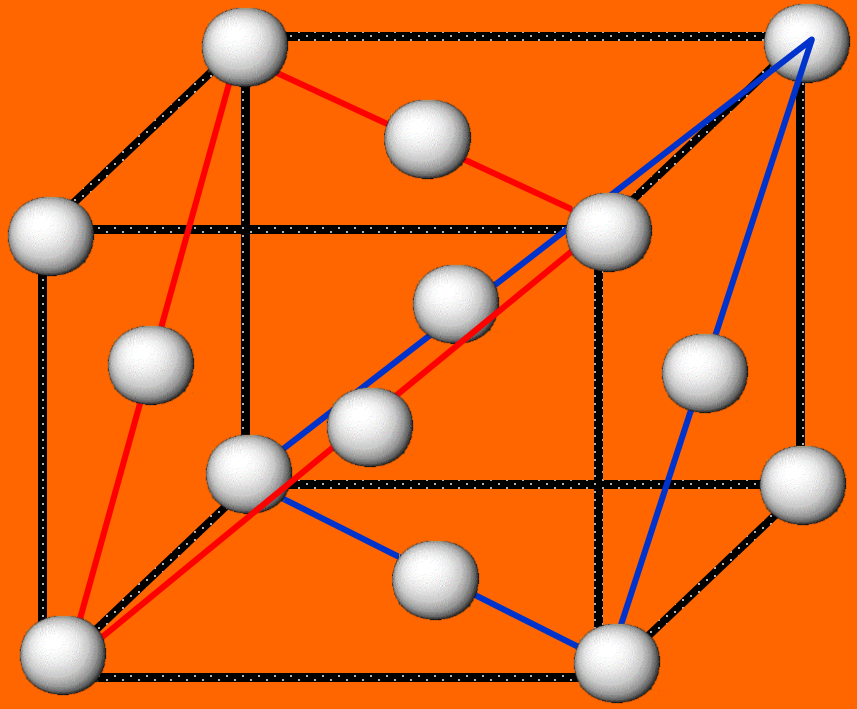
Layer B



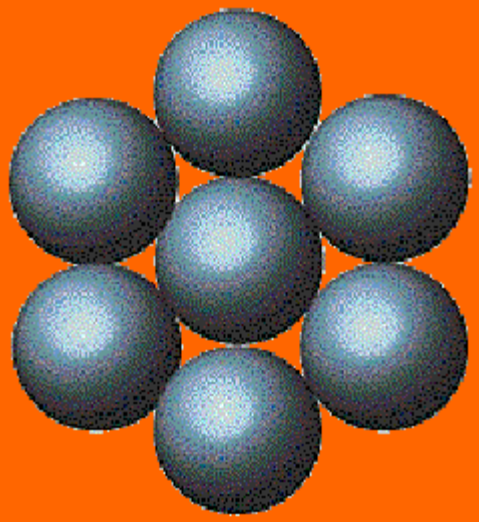
Layer C

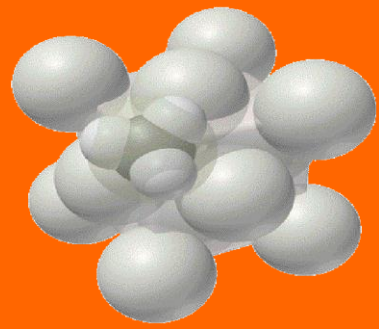




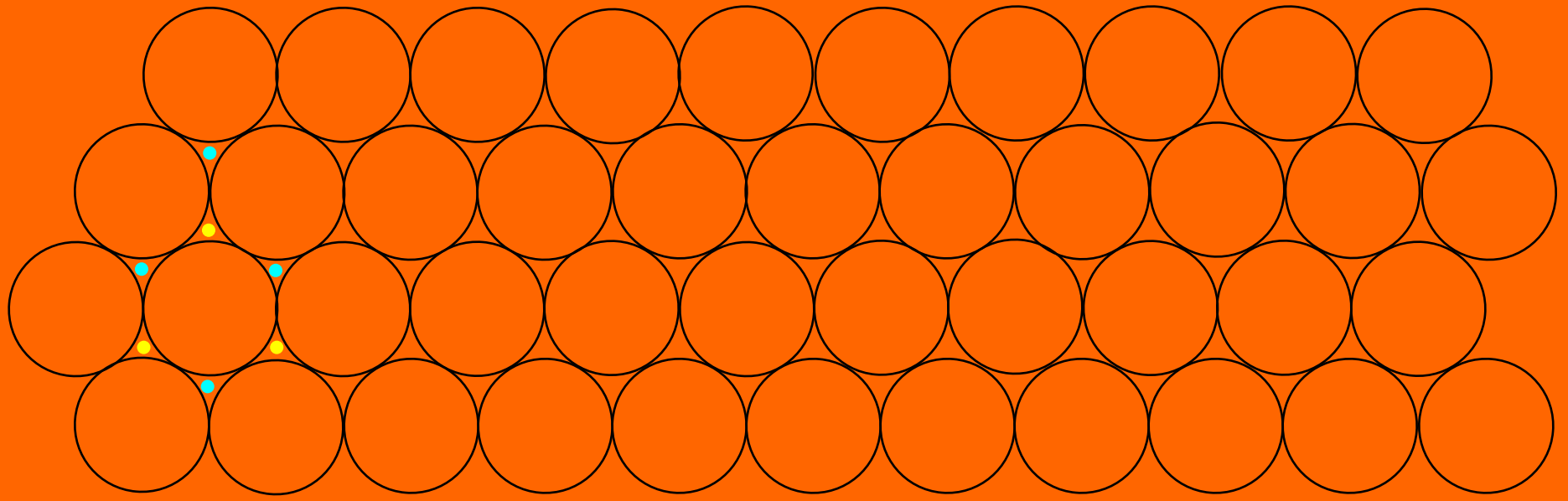


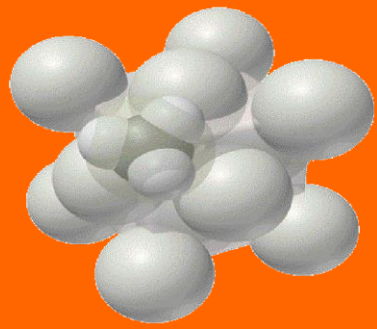
Layer arrangement view



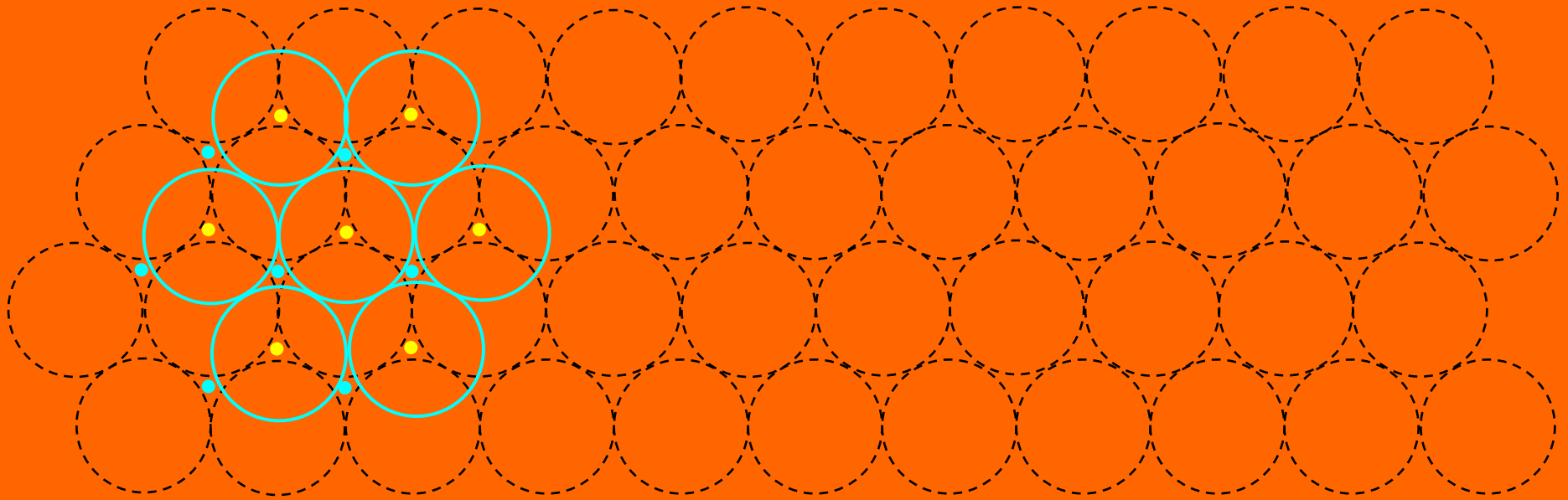


Layer A





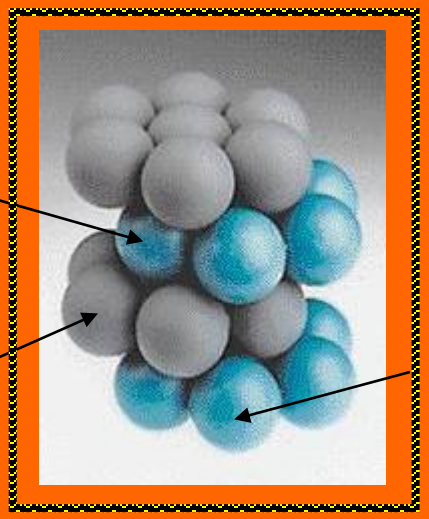
Layer B



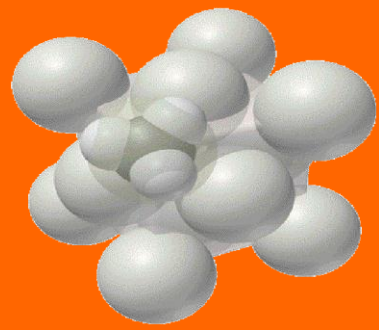
Layer A

Hexagonal Close Packing

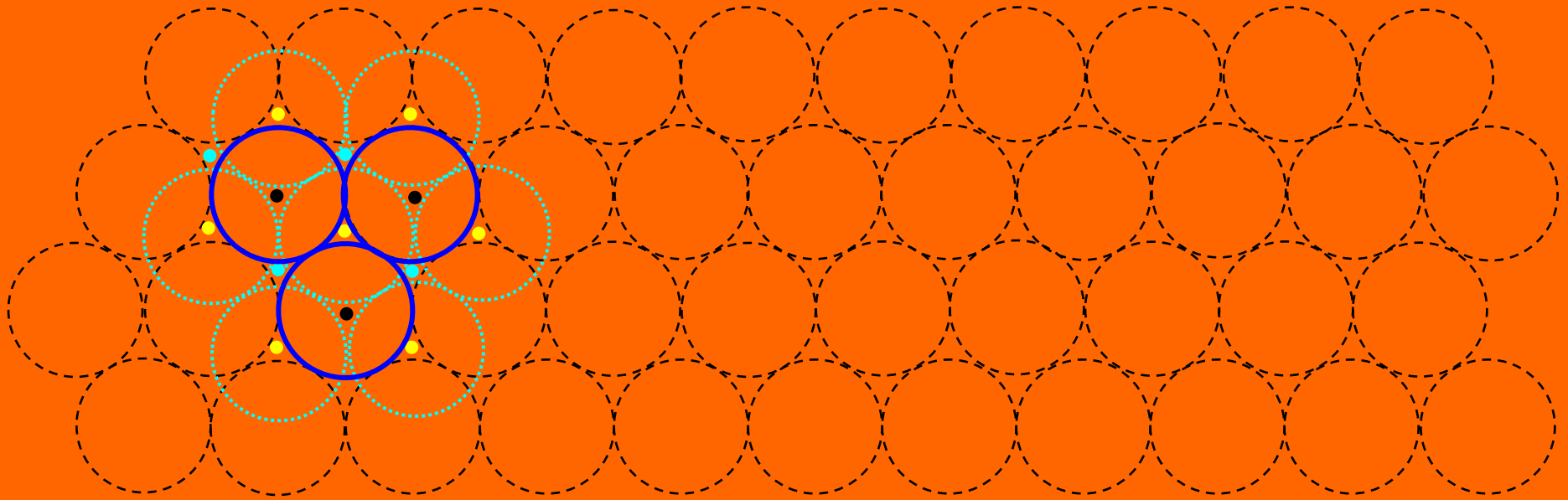
Layer B



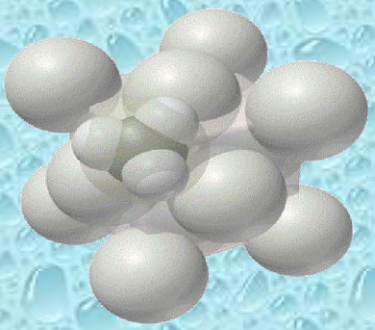
Layer A



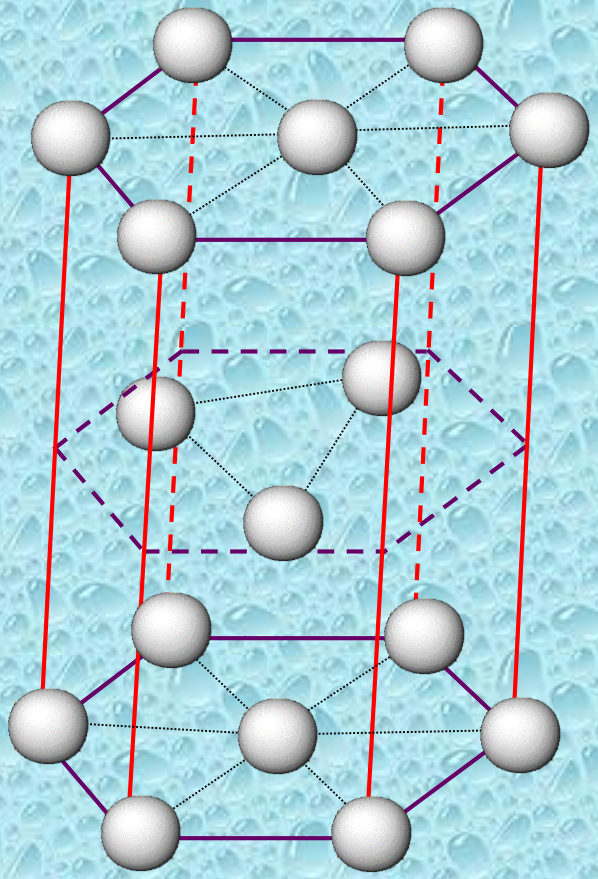
Layer A

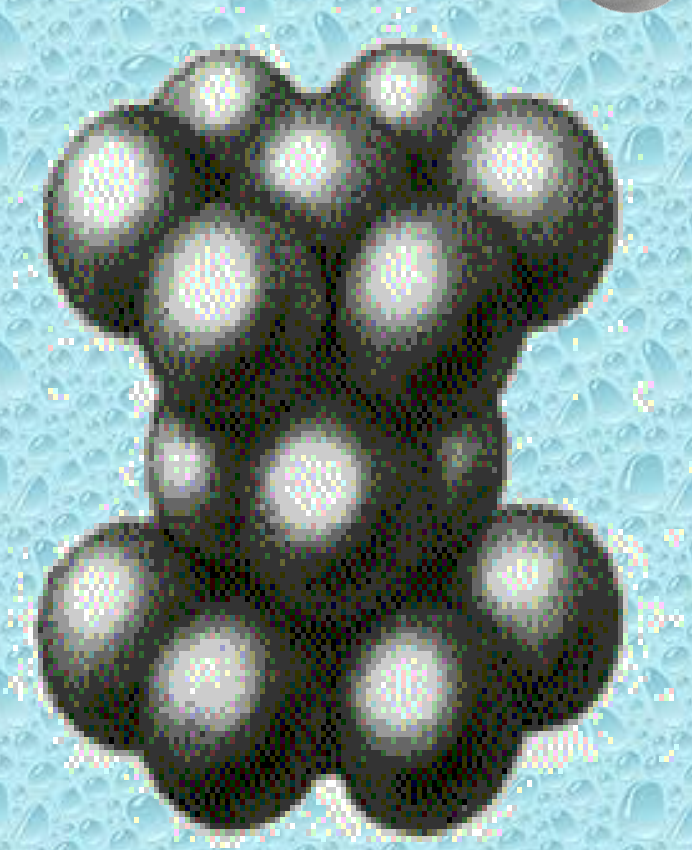


Hexagonal Primitive

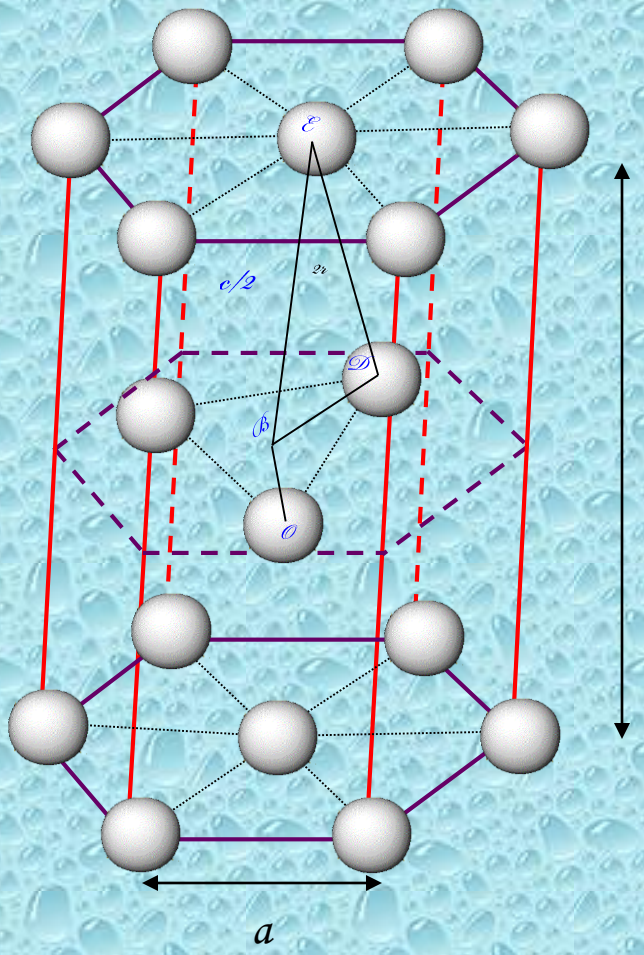


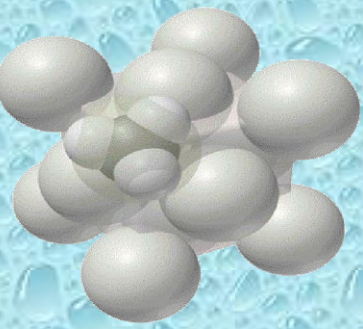
Unit Cell shape view



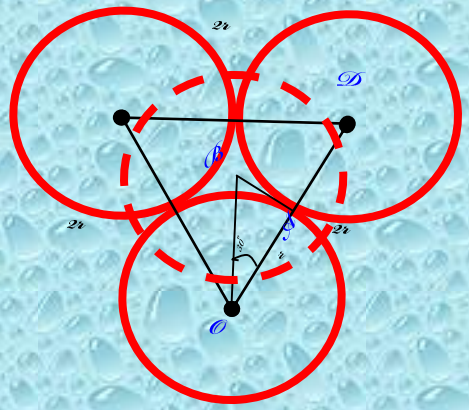


Unit Cell arrangement view





$a = 2r$



$OA = r$

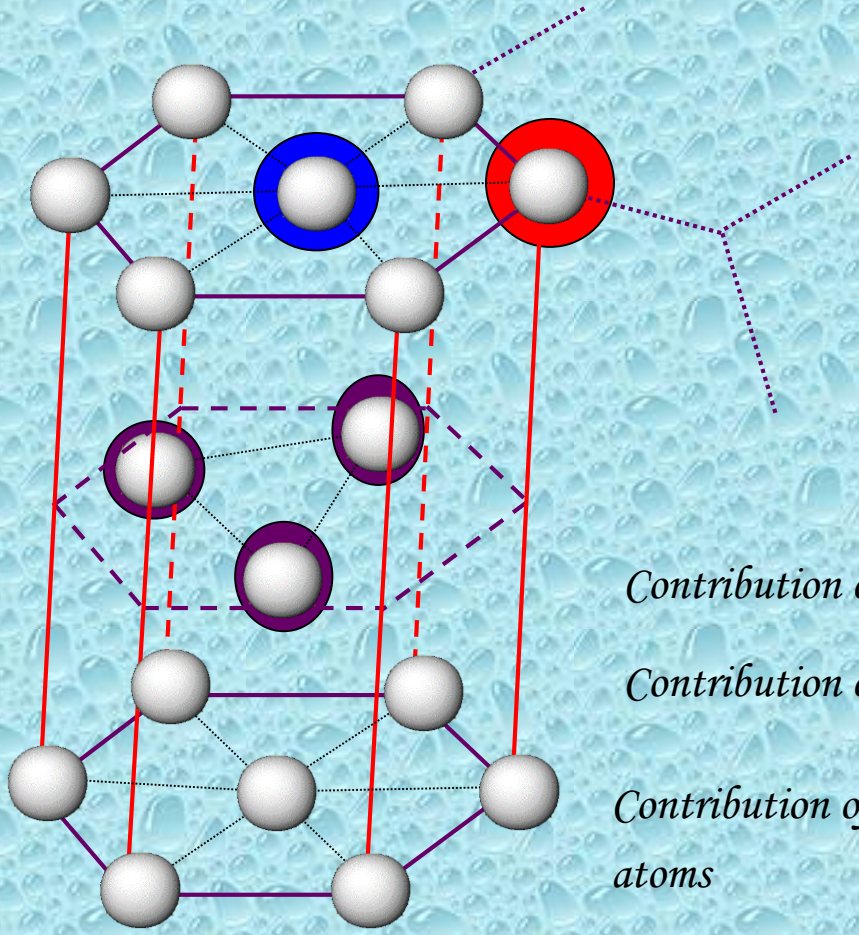
$\angle AOB = 30^o$

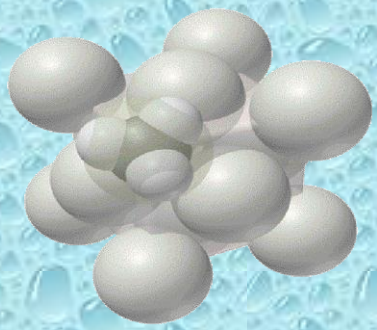
$$OB = \frac{2r}{\sqrt{3}} = BD$$

$$EB = \sqrt{(2r)^2 - \left(\frac{2r}{\sqrt{3}}\right)^2} = 2r\sqrt{\frac{2}{3}} = \frac{c}{2}$$

$$c = 4r\sqrt{\frac{2}{3}}$$

Hexagonal Primitive





Contribution of corner atom $= \frac{1}{6}$

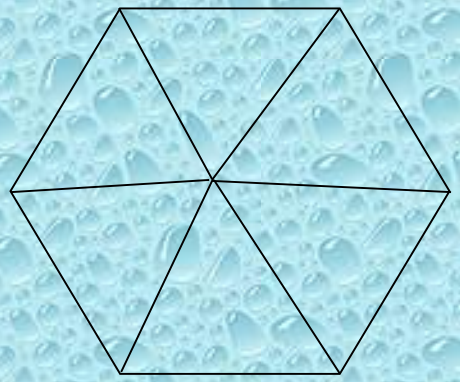
Contribution of Face atom $= \frac{1}{2}$

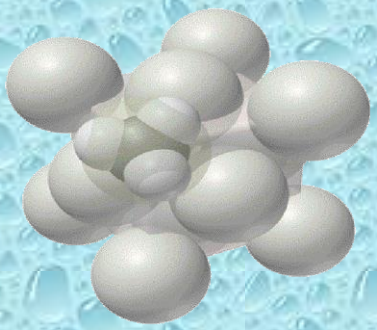
Contribution of second layer atoms $= 3$

Total atoms per unit cell $= 6$

Hexagonal Primitive

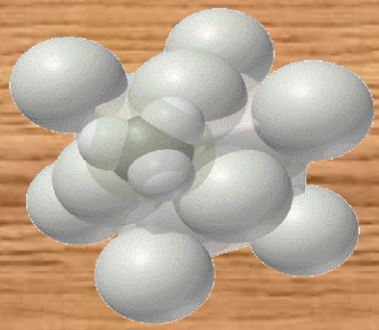
Packing Fraction





$$\frac{6\times\frac{4}{3}\pi r^3}{6\times\frac{\sqrt{3}}{4}(2r)^2\times 4r\sqrt{\frac{2}{3}}}=0.74$$

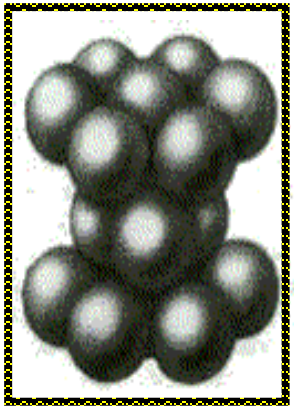
Hexagonal Primitive

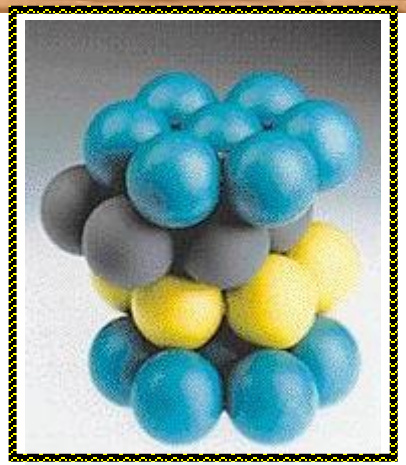


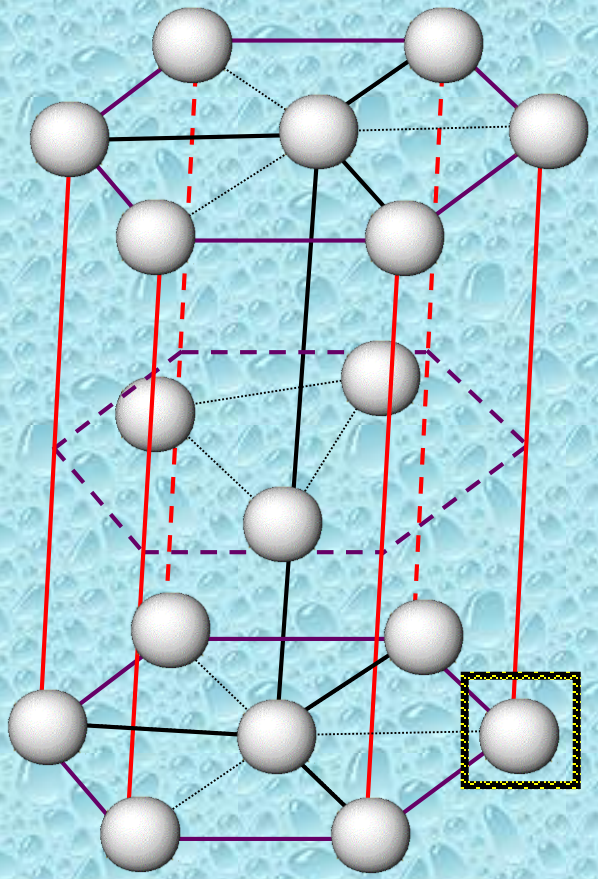
Packing Fraction depends on:

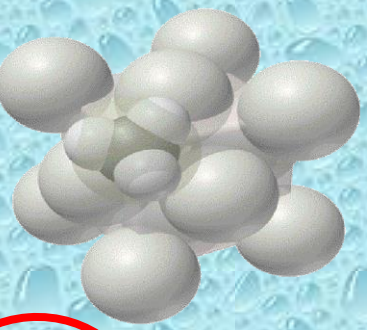
1. Layout of each layer

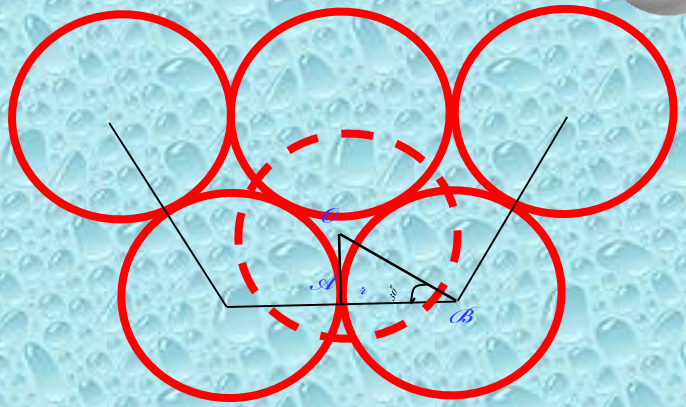
2. Placement of one layer over the other











$AB = r$

$OA = r \tan 30^o = \frac{r}{\sqrt{3}} < r$

Rank of unit cell – 2

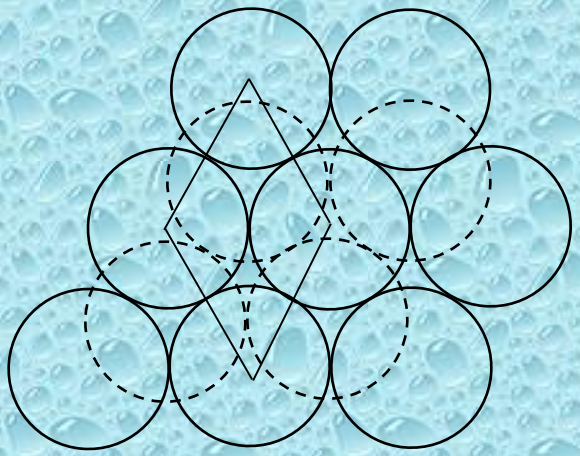
Volume of unit cell – 1/3 of previous

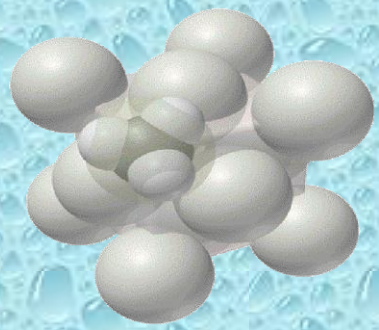
Packing Fraction – same

mass of unit cell – 1/3 of previous

density – same

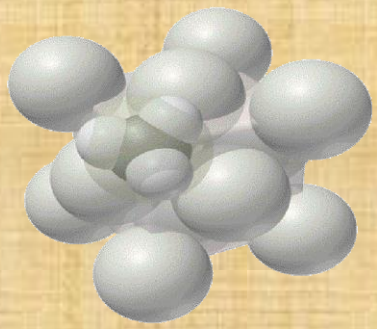
Hexagonal Primitive





Hexagonal Primitive

Voids



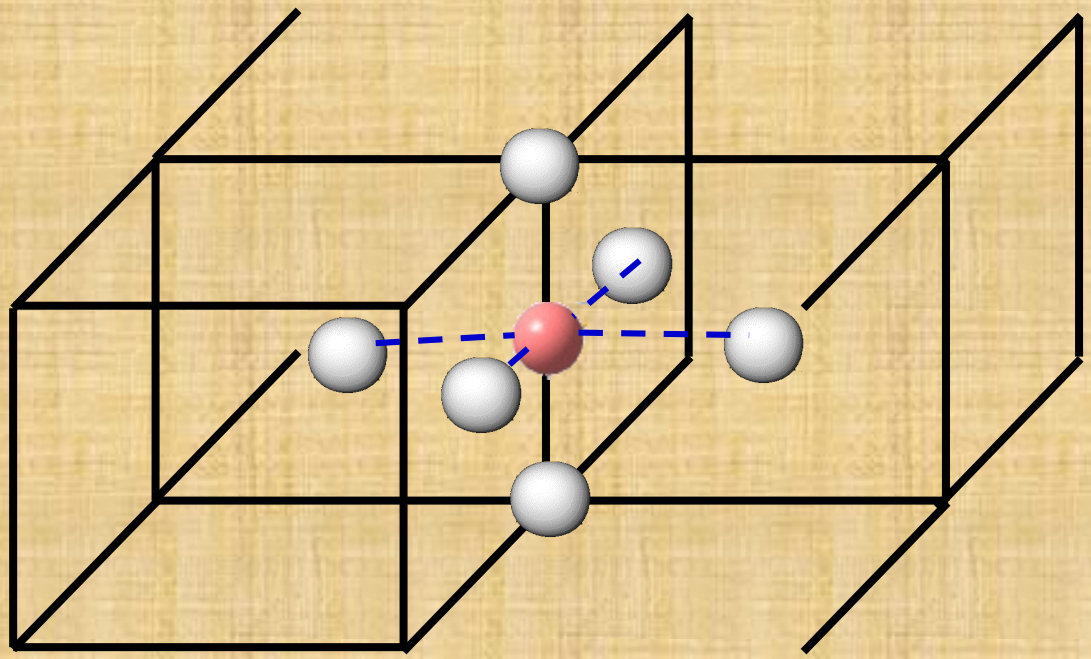
Two types of voids:

Octahedral

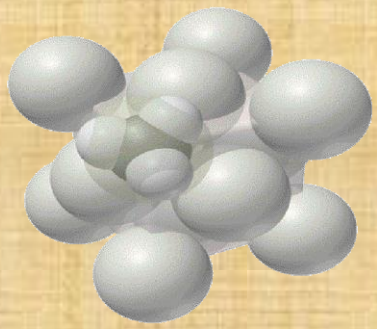
Tetrahedral

Found only in FCC & Hexagonal primitive unit cells

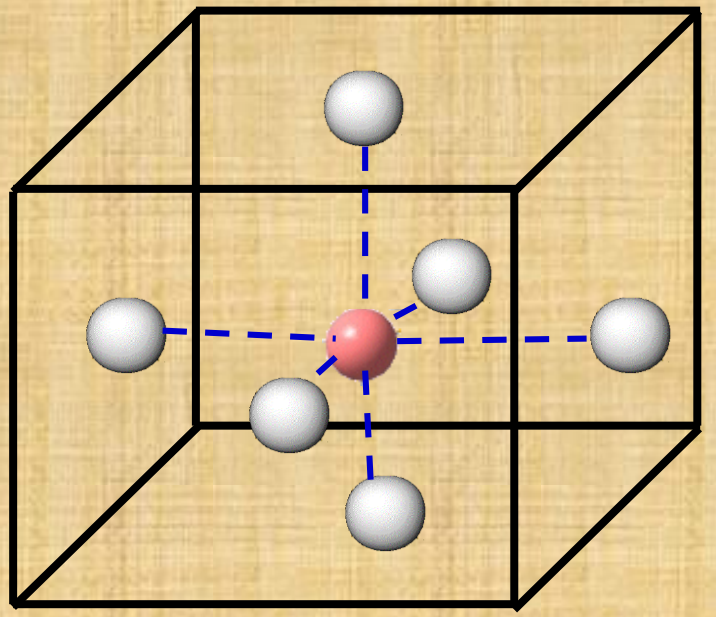
Octahedral void in FCC



Each octahedral void located at the edge center is shared by 4 unit cells



Total contribution of edge centre voids = $\frac{1}{4} \times 12 = 3$



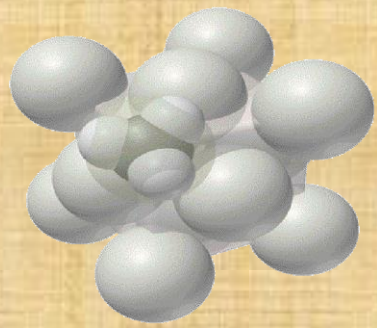
No. of Octahedral voids per unit cell = Rank of unit cell

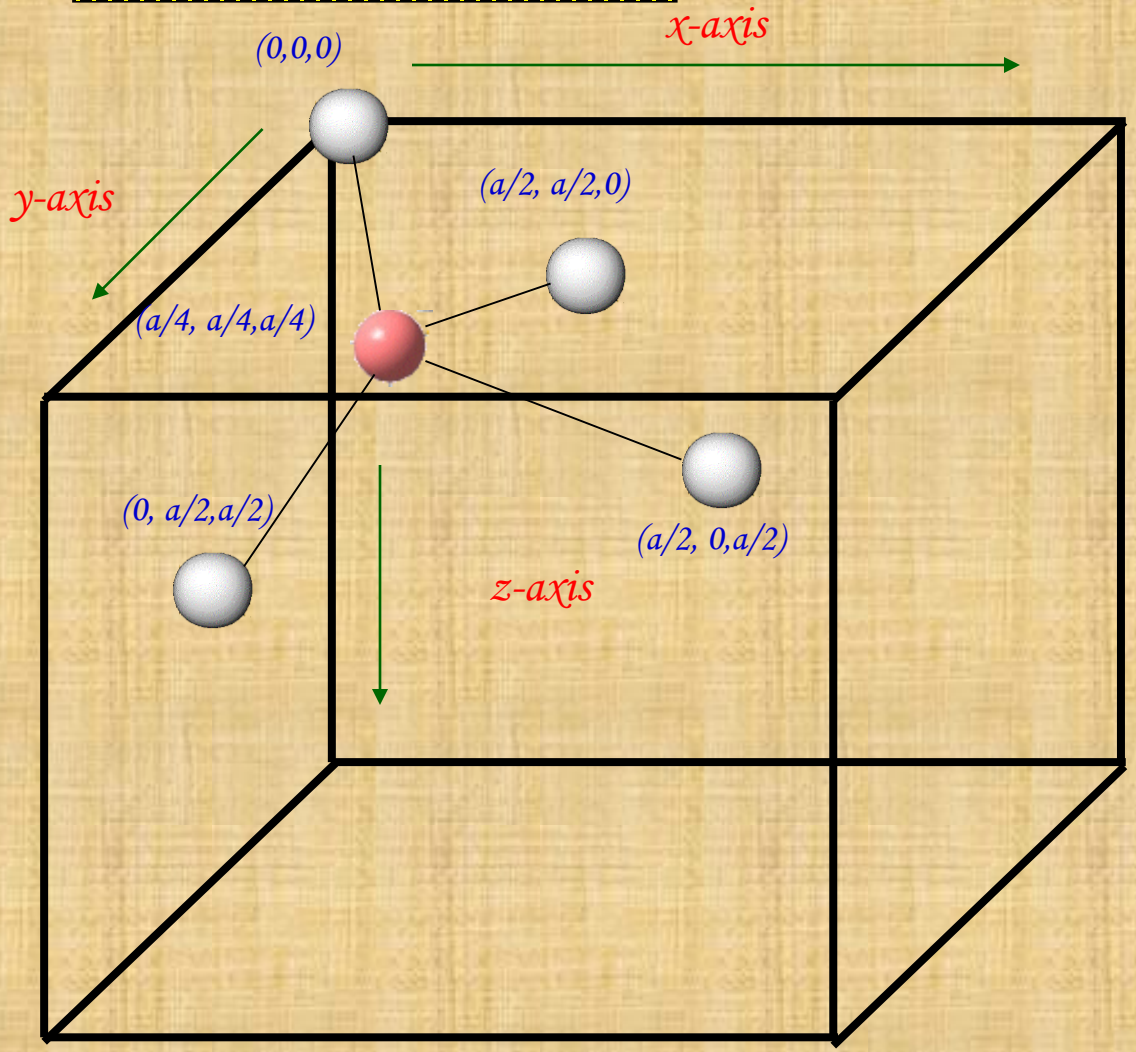
Contribution of central void $= 1$

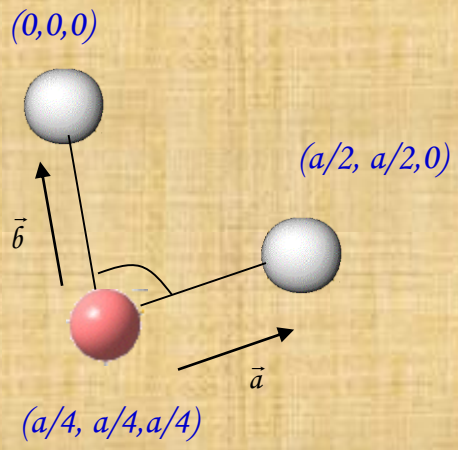
Total contribution of all octahedral voids per unit cell of FCC = 4

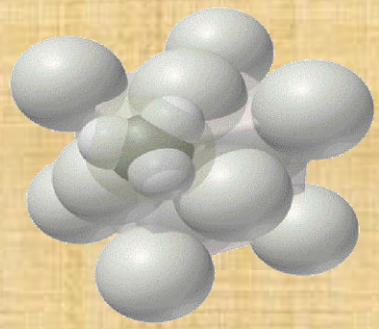
Voids

Tetrahedral void in FCC









$$\vec{a} = \frac{a}{4}\hat{i} + \frac{a}{4}\hat{j} - \frac{a}{4}\hat{k}$$

$$\vec{b} = -\frac{a}{4}\hat{i} - \frac{a}{4}\hat{j} - \frac{a}{4}\hat{k}$$

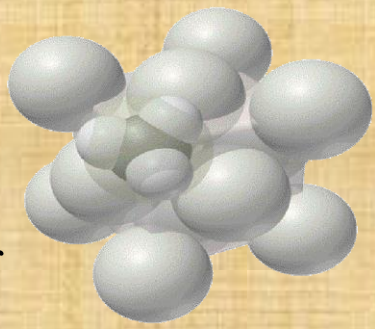
$$\cos^{-1}\left[\frac{\vec{a}.\vec{b}}{|\vec{a}|.|\vec{b}|}\right] = \theta$$

$$\cos^{-1}\left[\frac{-a^2/16}{3a^2/16}\right] = \theta$$

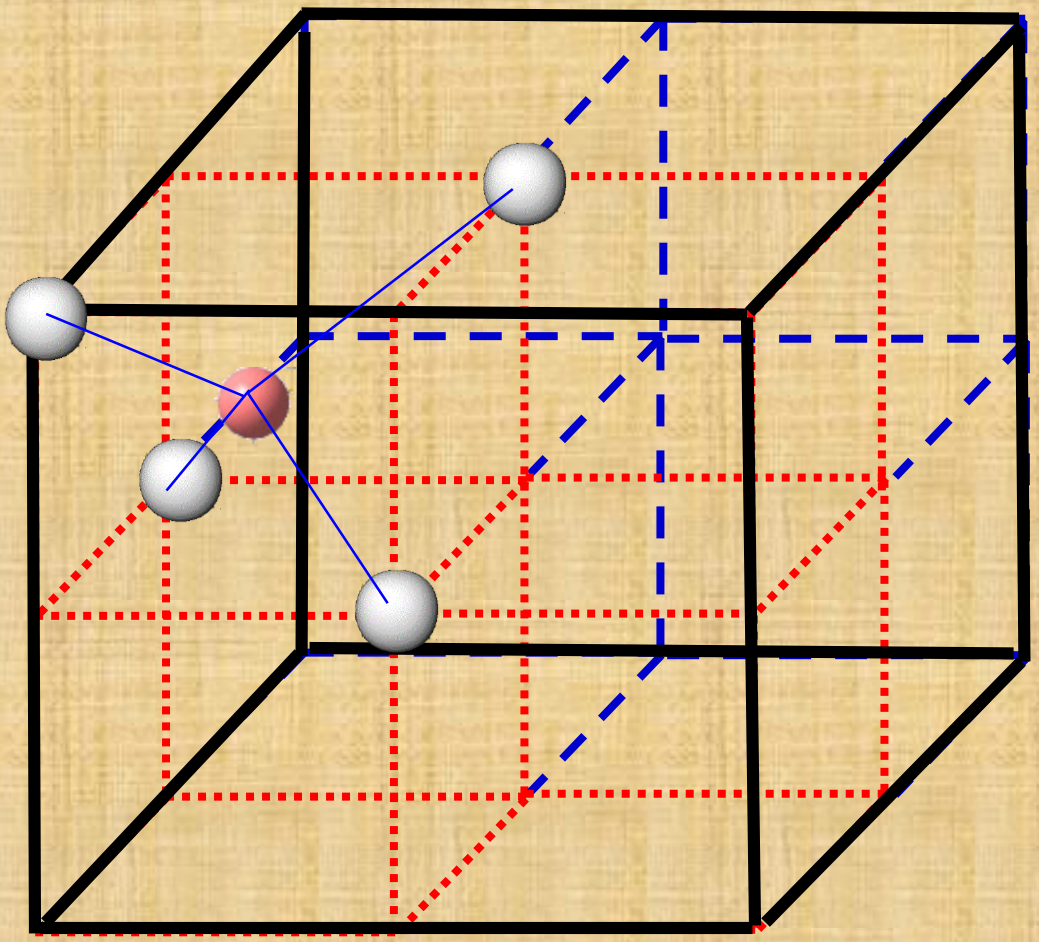
$$\cos^{-1}\left[-\frac{1}{3}\right] = \theta \qquad \theta = 109.268^{o}$$

Voids

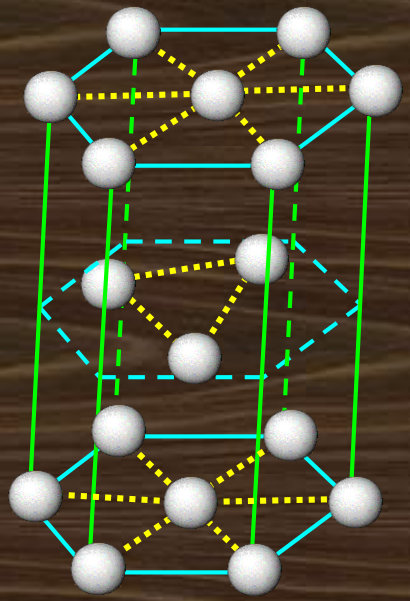
With each corner as origin there are 8 tetrahedral voids in FCC unit cell



$\therefore$ *No. of tetrahedral voids = 2 × no. of Octahedral voids*



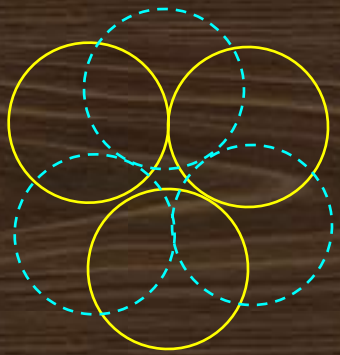
Voids in Hexagonal Primitive

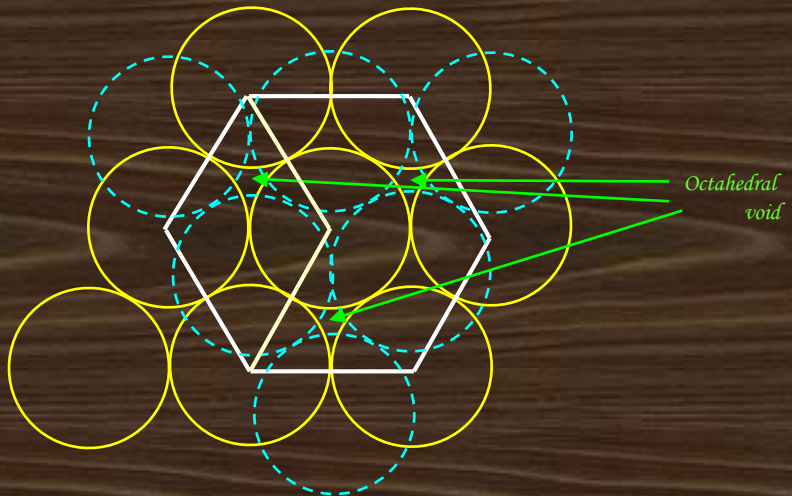


Let us assume that this is the unit cell

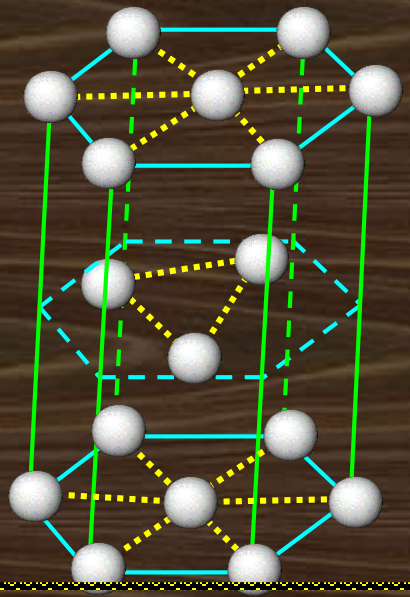
then according to what we have done in FCC no. of Octahedral voids = 6 & no. of tetrahedral voids = 12

Octahedral voids



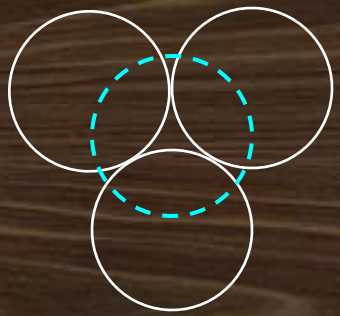


Voids in Hexagonal Primitive

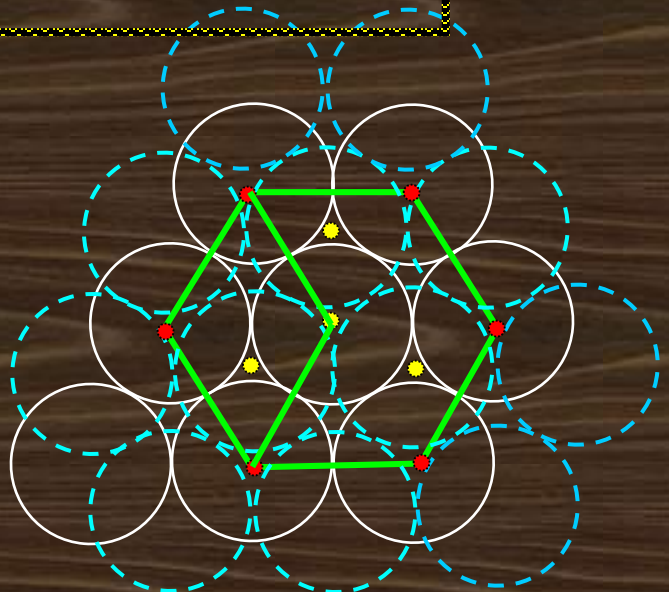


Let us assume that this is the unit cell

then according to what we have done in FCC no. of Octahedral voids = 6 & no. of tetrahedral voids = 12



Tetrahedral voids



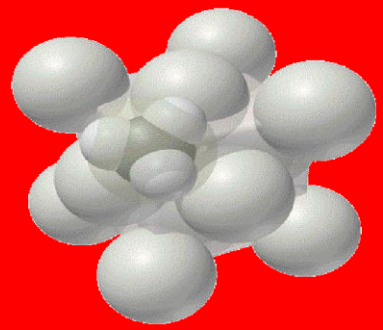
Contribution of tetrahedral voids formed inside the unit cell is 1 each. The ones formed on the corners of the hexagon have a contribution of 1/3.

Total contribution $= 4 + \frac{1}{3} \times 6 = 6$

In 3 layers $= 2 \times 6 = 12$

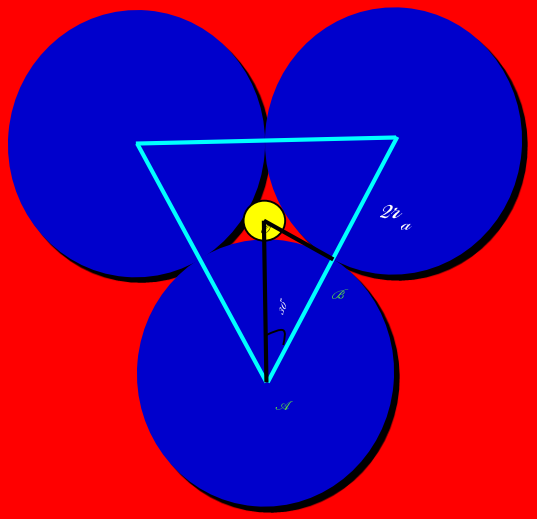
Voids

Radius Ratios



Minimum r_c/r_a for various coordination numbers

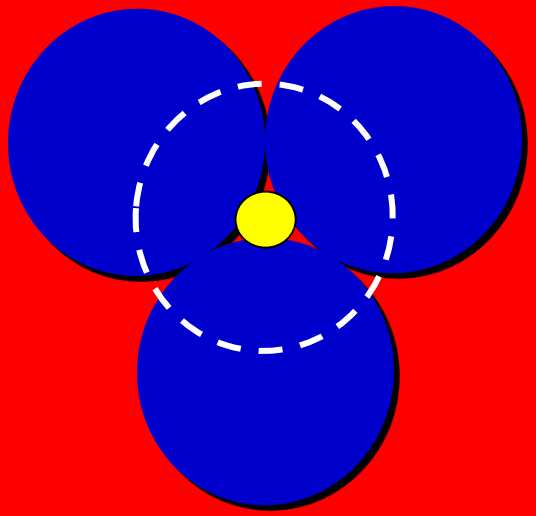
Coordination number - 3

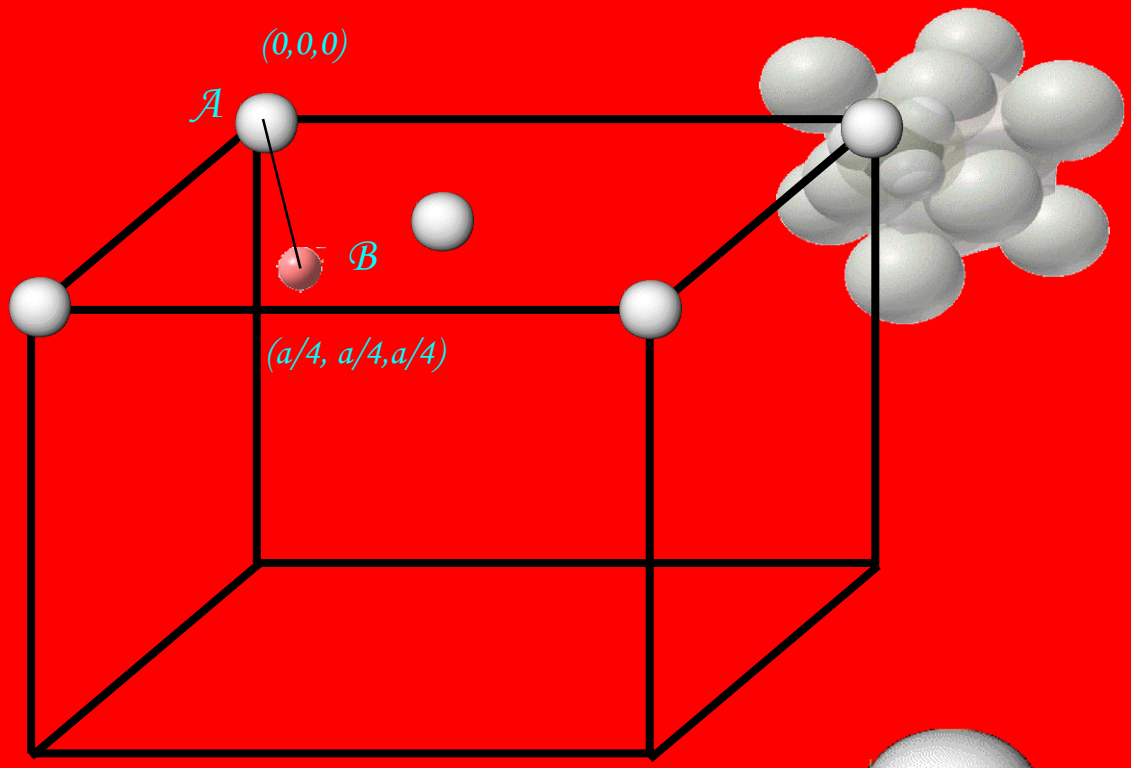


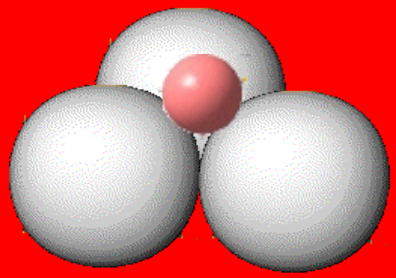
$$\frac{OA}{AB} = \frac{r_c + r_a}{r_a} = \sec 30^\circ = \frac{2}{\sqrt{3}}$$

$$\frac{r_c}{r_a} = \frac{2}{\sqrt{3}} - 1 = 0.155$$

Coordination number - 4







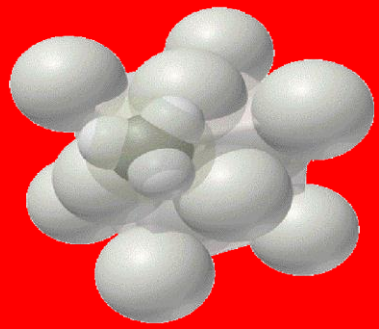
$$AB = r_c + r_a = \sqrt{\left(\frac{a}{4}\right)^2 + \left(\frac{a}{4}\right)^2 + \left(\frac{a}{4}\right)^2} = \frac{\sqrt{3}a}{4}$$

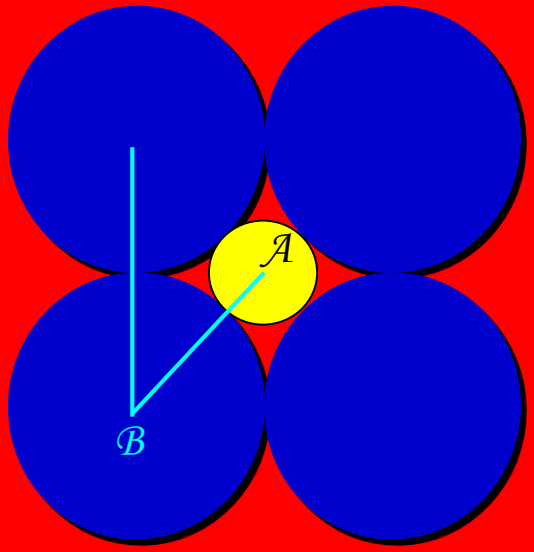
$$\sqrt{2}a = 4r_a$$

$$r_c + r_a = \frac{\sqrt{3}}{4}\left(\frac{4r_a}{\sqrt{2}}\right) \qquad r_c + r_a = \sqrt{\frac{3}{2}}r_a \qquad \frac{r_c}{r_a} + 1 = \sqrt{\frac{3}{2}} \qquad \frac{r_c}{r_a} = \sqrt{\frac{3}{2}} - 1 = 0.225$$

Radius Ratios

Coordination number - 4 (square planar) or 6 (octahedron)





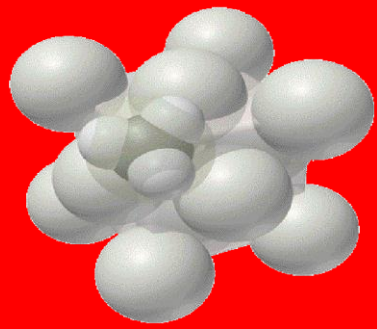
$$AB = r_c + r_a = \frac{a}{\sqrt{2}}$$

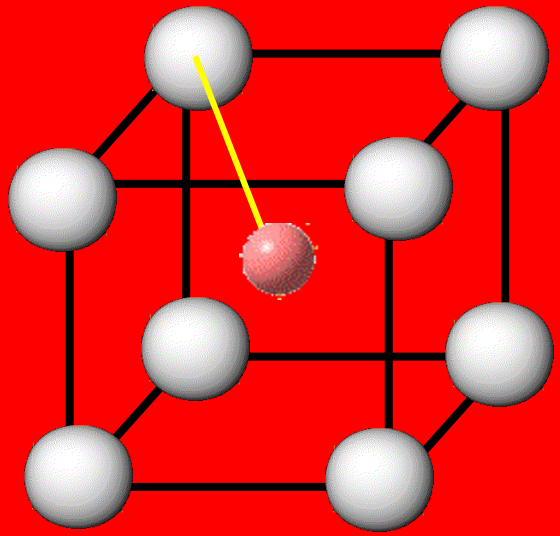
$$a = 2r_a$$

$$\therefore r_c + r_a = \frac{2r_a}{\sqrt{2}} = \sqrt{2}\, r_a$$

$$\therefore \frac{r_c}{r_a} = \sqrt{2} - 1 = 0.414$$

Coordination number - 8 (cube)





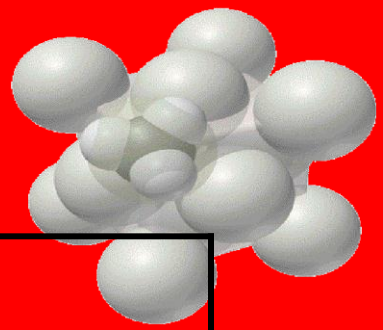
$$\frac{\sqrt{3}a}{2} = r_c + r_a$$

$$a = 2r_a$$

$$\frac{\sqrt{3}}{2} \times (2r_a) = r_c + r_a$$

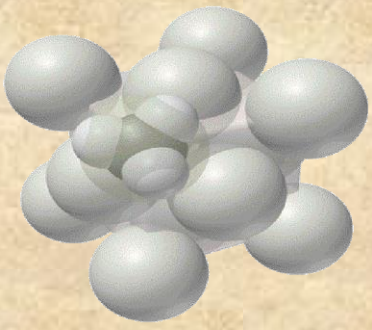
$$\therefore \frac{r_c}{r_a} = \sqrt{3} - 1 = 0.732$$

Final Radius Ratios



Radius Ratio, r_c/r_a	Co-ordination No.
<0.155	2
[0.155, 0.225)	2 or 3
[0.225, 0.414)	2 or 3 or 4 T_d
[0.414, 0.732)	2 or 3 or 4 T_d, 4 sq. pl or 6 O_h
[0.732, 0.99)	2 or 3 or 4 T_d, 4 sq. pl or 6 O_h or 8

Structures of Ionic Compounds

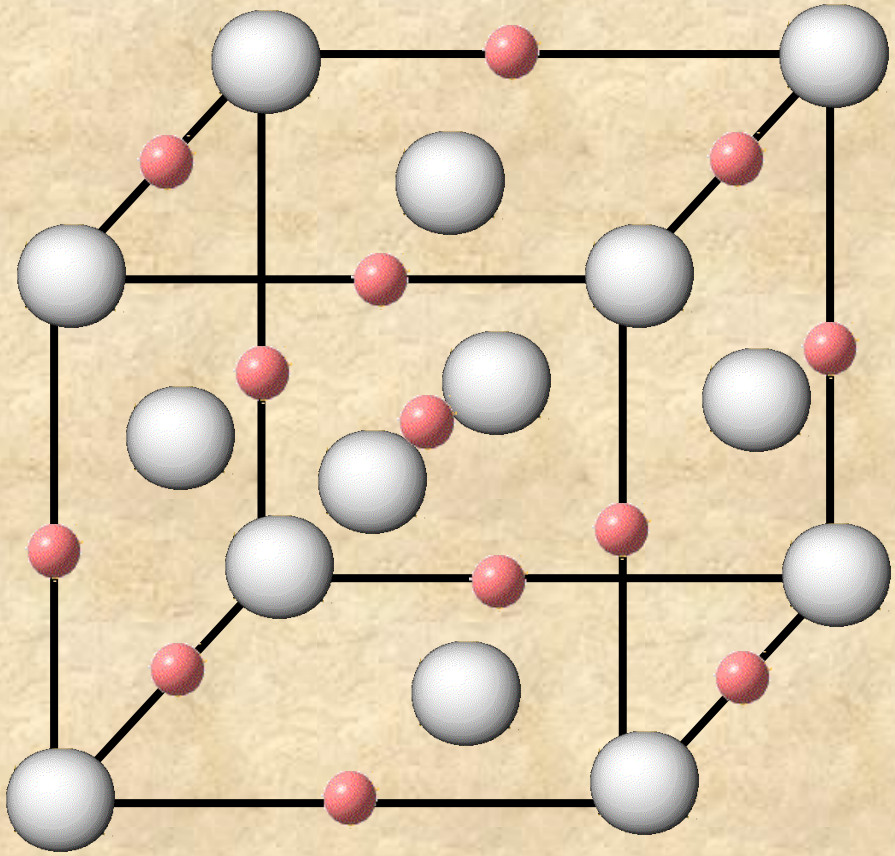


For ionic compounds of the general formula A_xB_y the ratio of the coordination number of A to that of B will be the ratio of y:x.

1. Rock Salt Structure (NaCl)

– Cl^-

– Na^+



Cl^- is FCC

Na^+ occupies Octahedral voids

No. of Cl^- per unit cell = 4

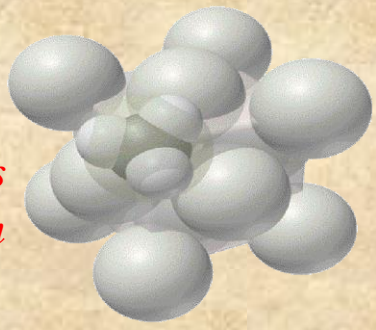
No. of Na^+ per unit cell = 4

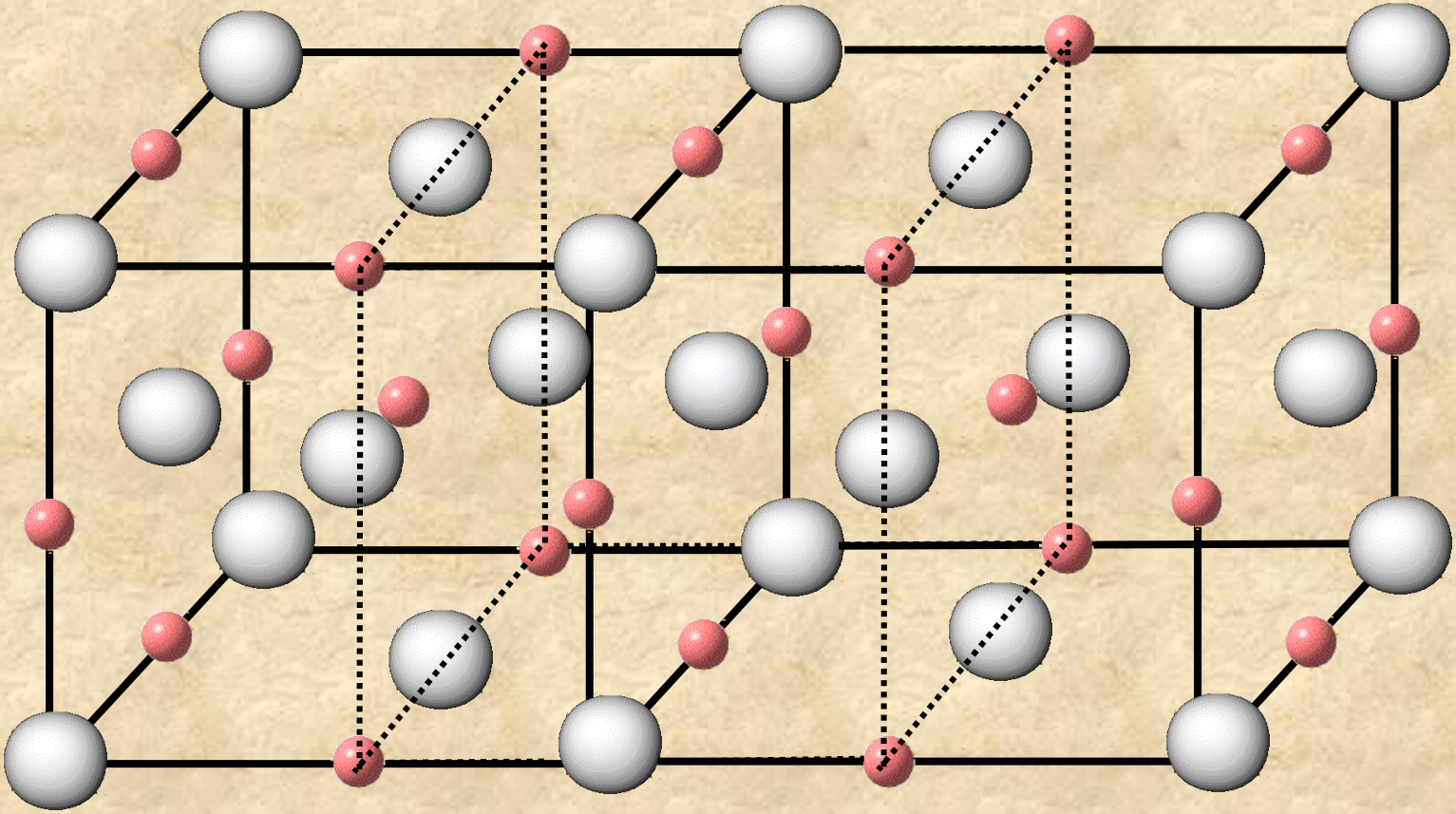
∴ formula is NaCl

Coordination no. of Na^+ = 6

Coordination no. of Cl^- = 6

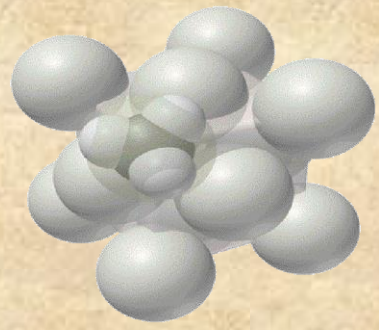
Other compounds which have this structure are: all halides of alkali metals except cesium halide, all oxides of alkaline earth metals except beryllium oxide, AgCl, AgBr & AgI.

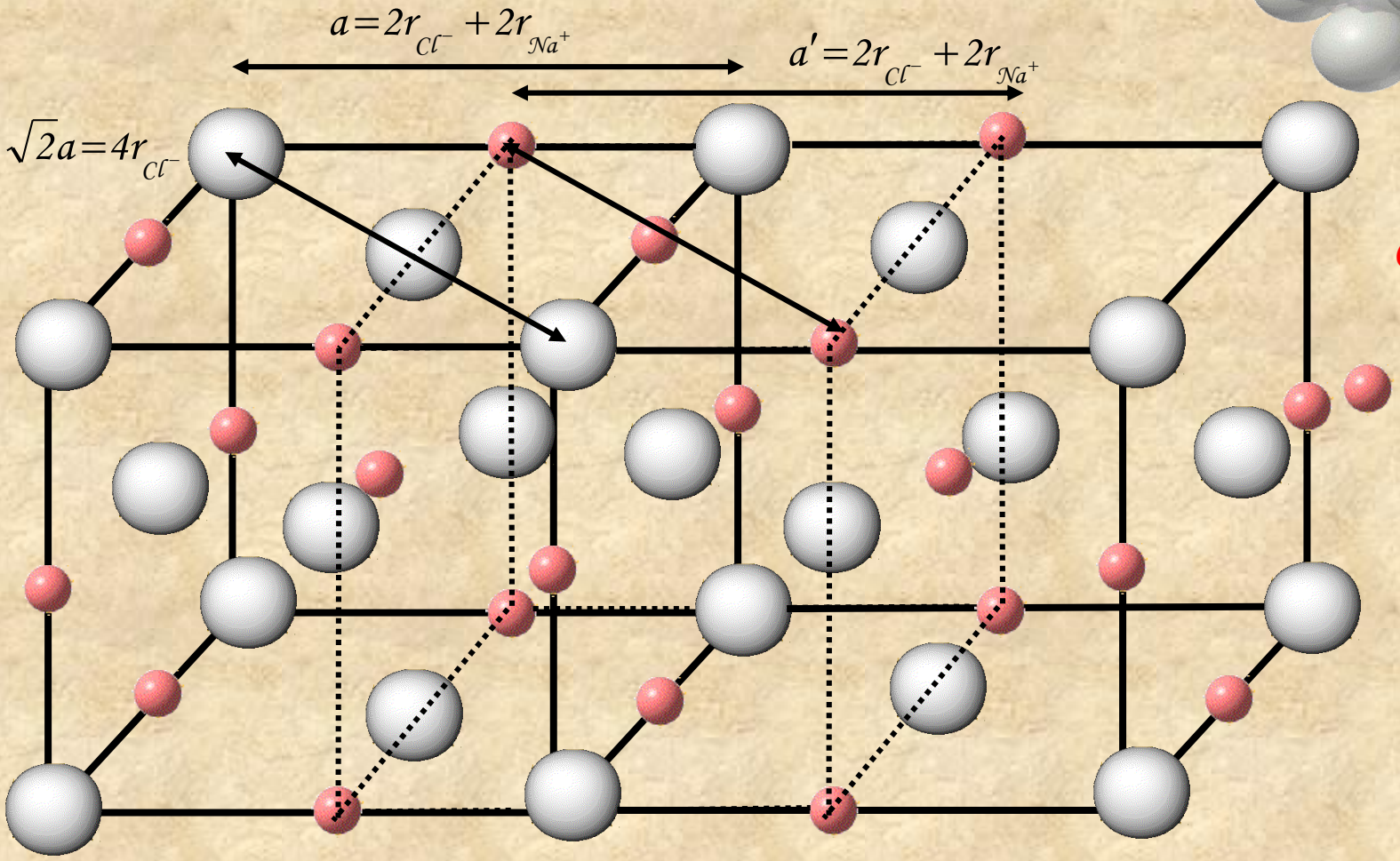




Consider the unit cell with Cl^- as FCC.

Consider the unit cell with Na^+ as FCC.





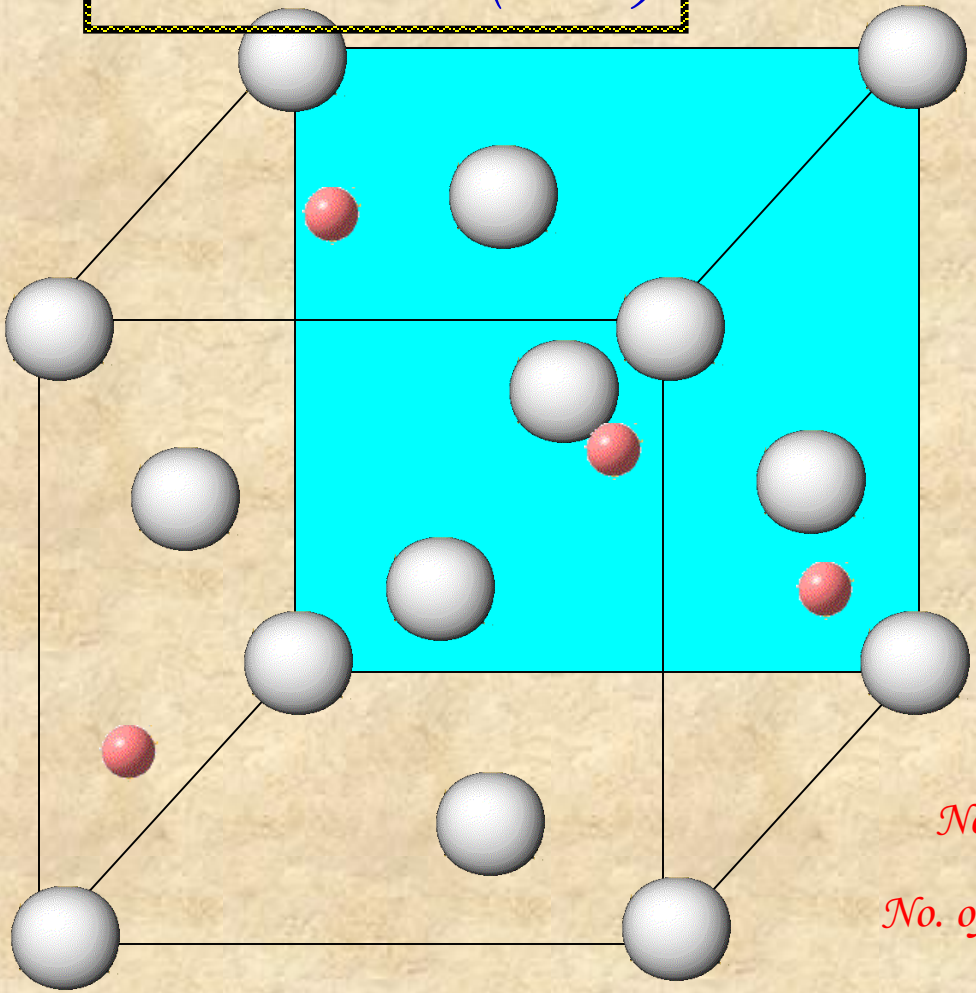
Comparing

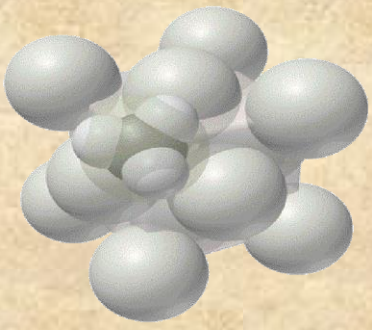
$r_{Na^+} = r_{Cl^-}$

Similarly, $r_{\text{any alkali metal}} = r_{\text{any halide}}$

$r_{\text{any akaline earth metal}} = r_{\text{oxide}}$

2. Zinc Blende (ZnS)





– S^{2-}

– Zn^{2+}

S^{2-} is FCC

Zn^{2+} occupies alternate tetrahedral voids

No. of S^{2-} per unit cell = 4

No. of Zn^{2+} per unit cell = 4

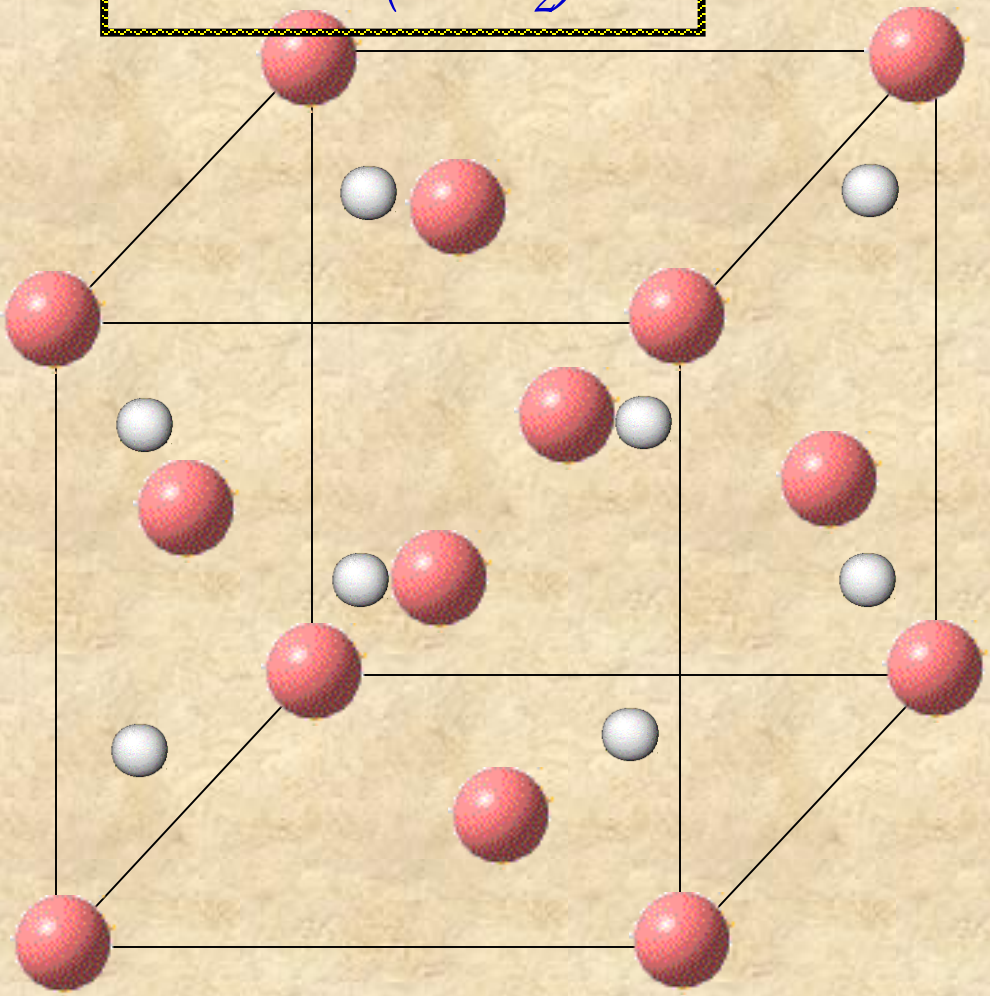
∴ formula is ZnS

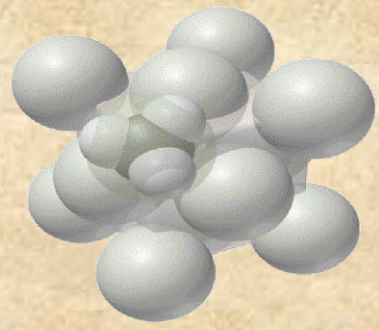
Coordination no. of Zn^{2+} = 4

Coordination no. of S^{2-} = 4

Other compound which have this structure is: BeO

3. Fluorite (CaF_2)





– F^-

– Ca^{2+}

Ca^{2+} is FCC

F^- occupies all tetrahedral voids

No. of Ca^{2+} per unit cell = 4

No. of F^- per unit cell = 8

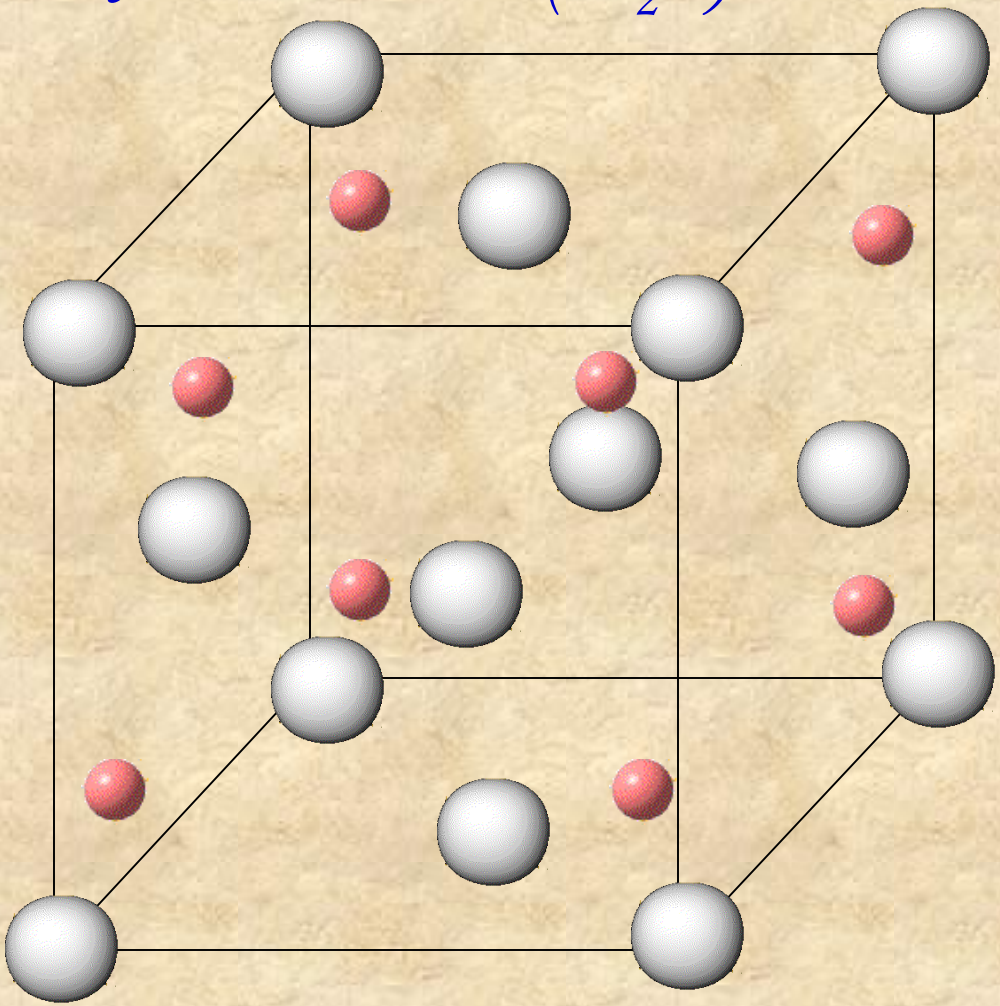
$\therefore$ formula is CaF_2

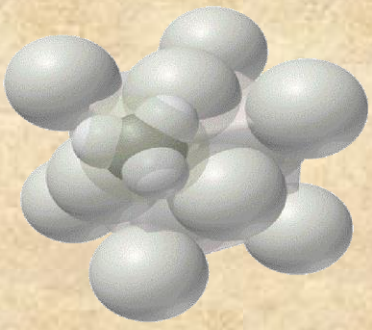
Other compounds which have this structure are: UO_2, ThO_2, PbO_2, HgF_2 etc.

Coordination no. of F^- = 4

Coordination no. of Ca^{2+} = 8

4. Anti-Fluorite (Li_2O)





– O^{2-}

– Li^+

O^{2-} is FCC

Li^+ occupies all tetrahedral voids

No. of O^{2-} per unit cell = 4

No. of Li^+ per unit cell = 8

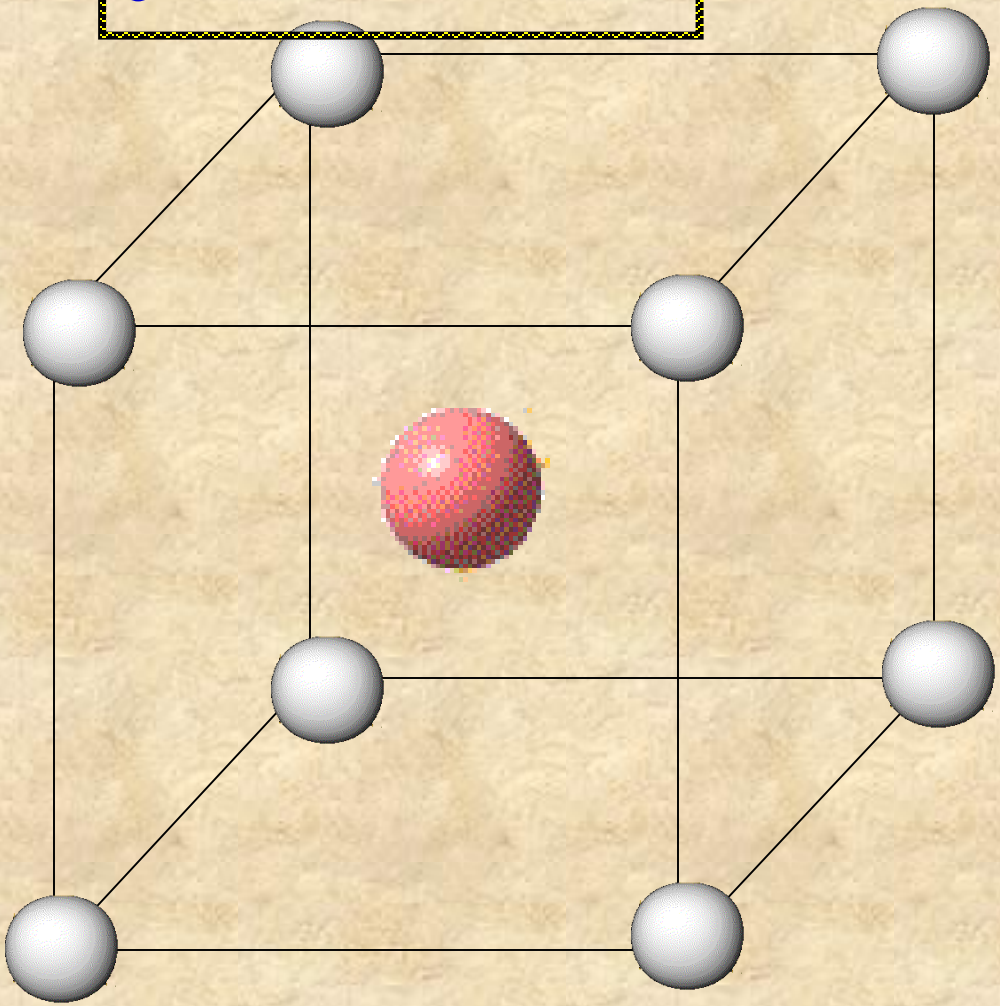
$\therefore$ formula is Li_2O

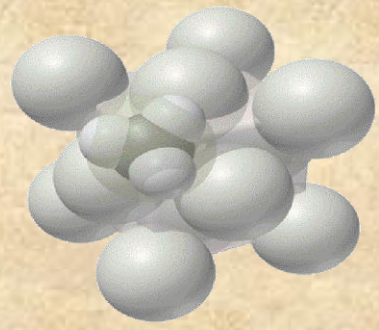
Other compounds which have this structure are: Na_2O, K_2O, Rb_2O

Coordination no. of Li^+ = 4

Coordination no. of O^{2-} = 8

5. Cesium Halide





– Cl^-

– Cs^+

Cl^- is Primitive cubic

Cs^+ occupies the centre of the unit cell

No. of Cl^- per unit cell = 1

No. of Cs^+ per unit cell = 1

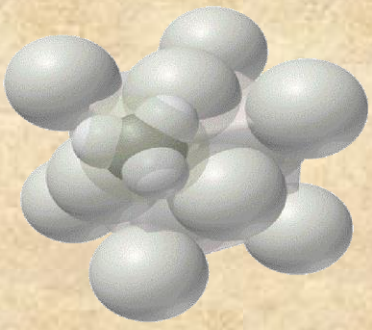
∴ formula is CsCl

Other compounds which have this structure are: all halides of Cesium and ammonium

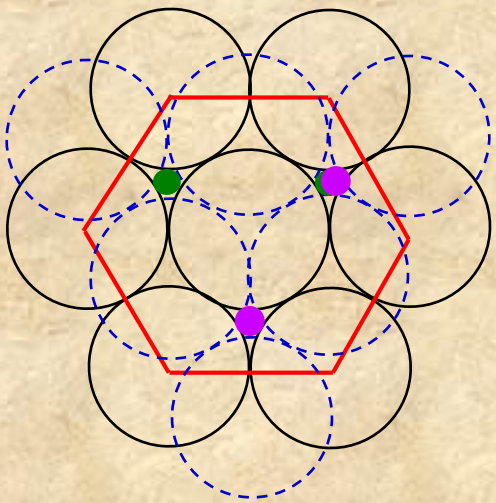
Coordination no. of Cs^+ = 8

Coordination no. of Cl^- = 8

6. Corundum (Al_2O_3)



Oxide ions form hexagonal primitive unit cell and trivalent ions (Al^{3+}) are present in 2/3 of octahedral voids.



No. of O^{2-} per unit cell = 2

No. of Al^{3+} per unit cell = 4/3

$\therefore$ formula is $Al_{\frac{4}{3}}O_2$; Al_4O_6

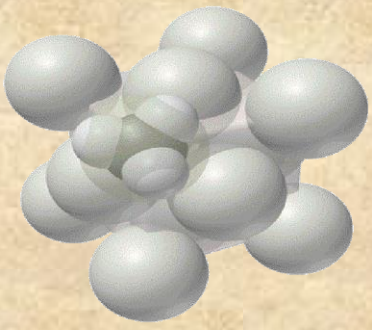
Al_2O_3

Coordination no. of Al^{3+} = 6

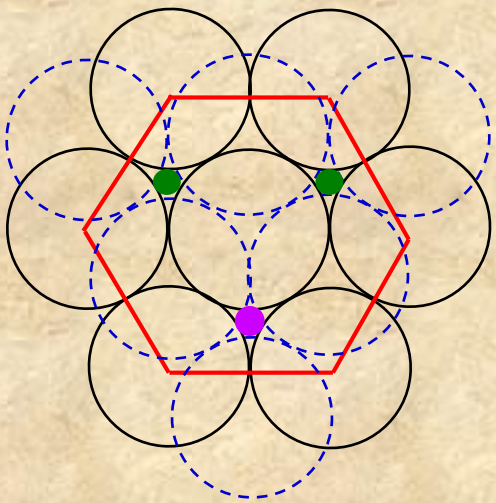
Coordination no. of O^{2-} = 4

Other compounds which have this structure are: Fe_2O_3, Cr_2O_3, Mn_2O_3 etc.

7. Rutile (TiO_2)



Oxide ions form hexagonal primitive unit cell and tetravalent ions (Ti^{4+}) are present in 1/2 of octahedral voids.



No. of O^{2-} per unit cell = 2

No. of Ti^{4+} per unit cell = 1

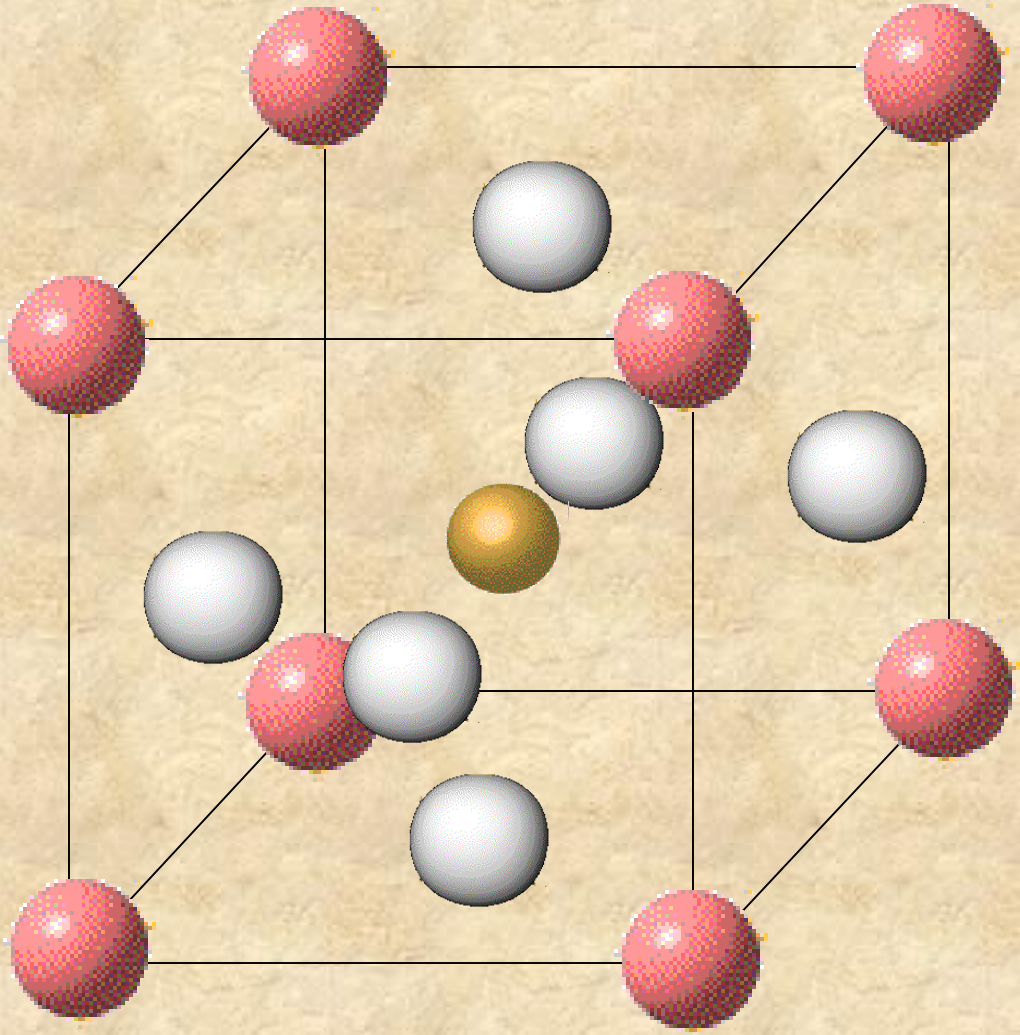
$\therefore$ formula is TiO_2

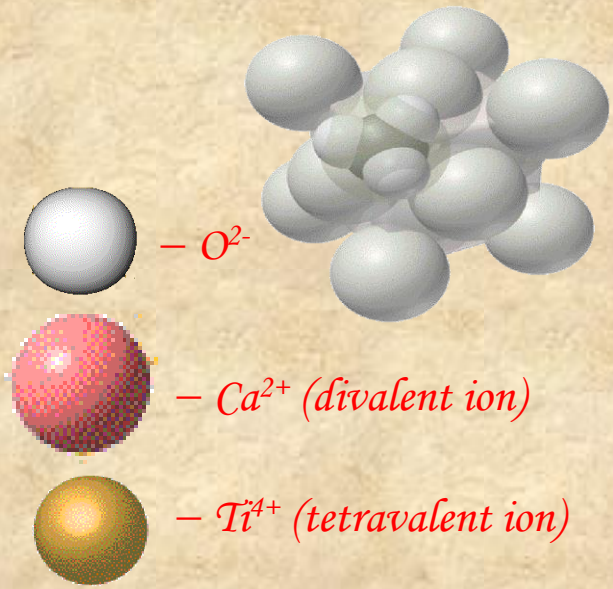
Coordination no. of Ti^{4+} = 6

Coordination no. of O^{2-} = 3

Other compounds which have this structure are: MnO_2, SnO_2, MgF_2, NiF_2

8. Pervoskite ($CaTiO_3$)





Ca^{2+} is Primitive cubic

Ti^{4+} occupies the centre of the unit cell

O^{2-} occupies face centres

No. of O^{2-} per unit cell = 3

No. of Ca^{2+} per unit cell = 1

No. of Ti^{4+} per unit cell = 1

$\therefore$ formula is $CaTiO_3$

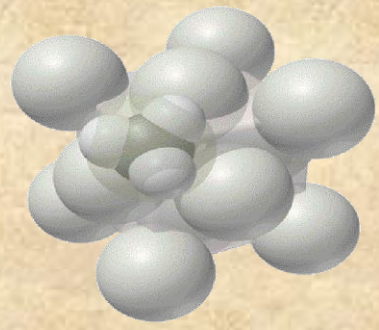
Coordination no. of O^{2-} = 6

Coordination no. of Ti^{4+} = 6

Coordination no. of Ca^{2+} = 12

Other compounds which have this structure are: $BaTiO_3$, $SrTiO_3$

9. Spinel & Inverse Spinel ($MgAl_2O_4$)



Spinel

O^{2-} ion is FCC

Mg^{2+} (divalent ion) $1/8^{th}$ of tetrahedral voids

Al^{3+} (trivalent ion) 1/2 of octahedral voids

O^{2-} per unit cell = 4

Mg^{2+} per unit cell = 1

Al^{3+} per unit cell = 1

$\therefore$ formula is $MgAl_2O_4$

Inverse Spinel

O^{2-} ion is FCC

divalent ion $1/8^{th}$ of tetrahedral voids

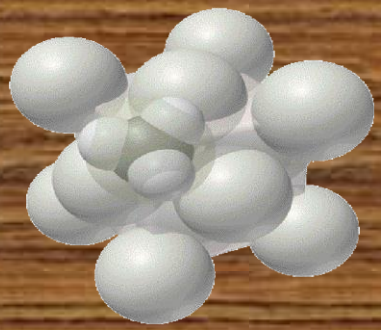
trivalent ion $1/4^{th}$ of octahedral voids & $1/8^{th}$ of tetrahedral voids

O^{2-} per unit cell = 4

Divalent per unit cell = 1

Trivalent per unit cell = 1

Crystal Defects



(i) Lattice of atoms

(a) Vacancy – an atom is missing from its position
– density decreases
– percentage occupancy decreases

$$\%\,occpancy = \frac{no.\,of\ atoms\ present}{no.\,of\ atoms\ present\,without\,defect} \times 100$$

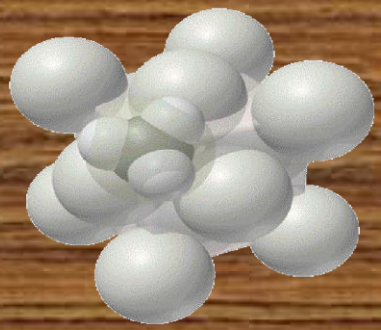
$$\%\,occpancy = \frac{observed\ density}{theoretical\ density} \times 100$$

(b) Self interstitial – an atom leaves its lattice site & occupies interstitial space
– density & percentage occupancy remains same

(c) Substitutional impurity – foreign atom substitutes a host atom & occupies its lattice
– density & percentage occupancy may change

(c) Interstitial impurity – foreign atom occupies occupies the interstitial space
– density & percentage occupancy increases

Crystal Defects



(i) Ionic structures

(a) Schottky Defect
- Cation – anion pair are missing
- electro neutrality is maintained
- density decreases

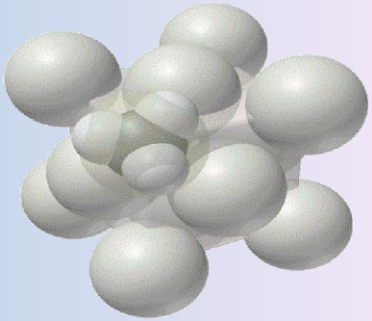
(a) F-Centre
- electron replaces anion
- electro neutrality is maintained
- density decreases
- colour is imparted

(b) Frenkel Defect
- ion leaves lattice position & occupies interstitial space
- electro neutrality is maintained
- density maintained

(c) Substitutional Impurity Defect
- Ba^{2+} is replaced by Sr^{2+}
- electro neutrality is maintained
- density changes

(d) Interstitial Impurity Defect
- H_2 is trapped in TiC
- electro neutrality is maintained
- density increases

1. *Assuming diamond to be FCC of carbon atoms and that each carbon atom is sp^3 hybridized then which of the following statements is correct.*



(a) all voids are empty

(b) 100% octahedral voids are filled

(c) 50% octahedral voids are filled

(d) 100% tetrahedral voids are filled

(e) 50% tetrahedral voids are filled

Sol: If no void is filled then each carbon would be in contact with 12 carbon atoms. This is not possible as each carbon is sp^3 hybridized.

If octahedral voids are filled then those carbons in the voids would be in contact with 6 carbon atoms. This also is not possible.

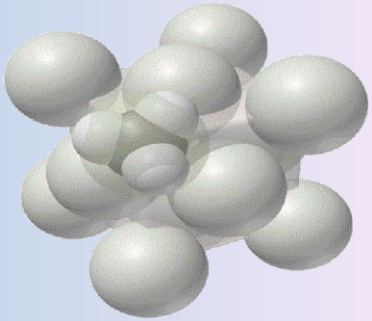
If 100% tetrahedral voids are filled then the FCC carbons would be in contact with 8 carbon atoms as they are shared in 8 unit cells and would be in contact with 8 tetrahedral voids. Not possible.

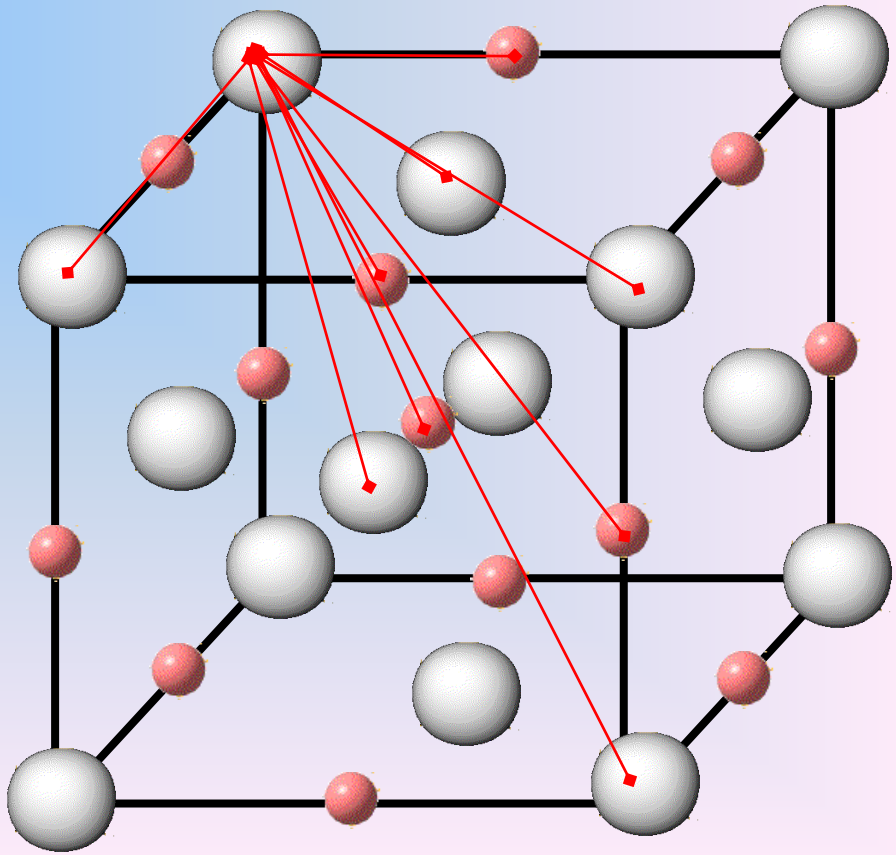
$\therefore$ (e)

2. *In NaCl calculate:*

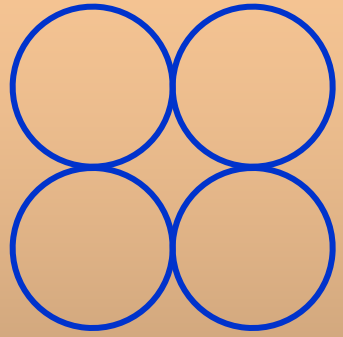
The distance between the first 9 nearest neighbors in a unit cell & their total number in all unit cells

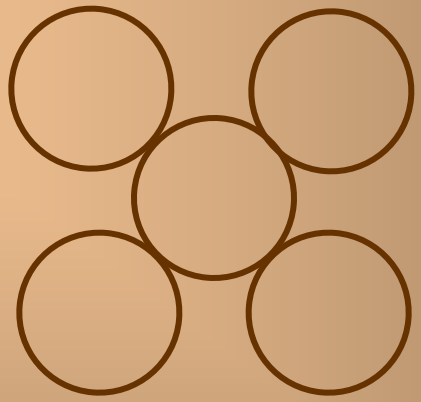
neighbor no.	distance	no. of neighbors
1	$\frac{a}{2}$	6
2	$\frac{a}{\sqrt{2}}$	12
3	$\frac{\sqrt{3}a}{2}$	8
4	a	6
5	$\frac{\sqrt{5}a}{2}$	24
6	$\sqrt{\frac{3}{2}}a$	24
7	$\sqrt{2}a$	12
8	$\frac{3}{2}a$	24
9	$\sqrt{3}a$	8

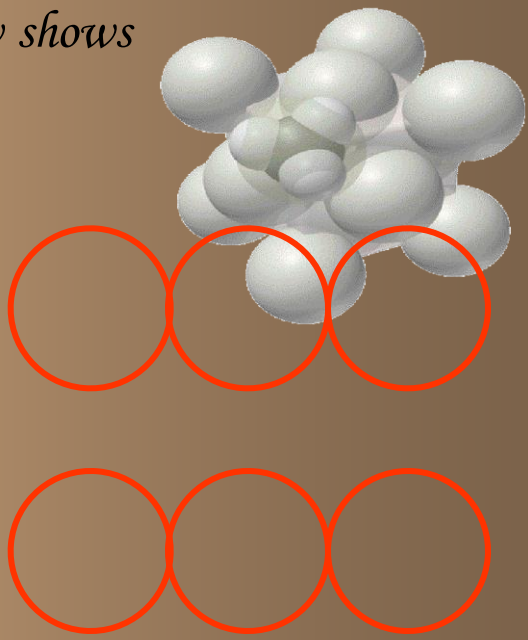


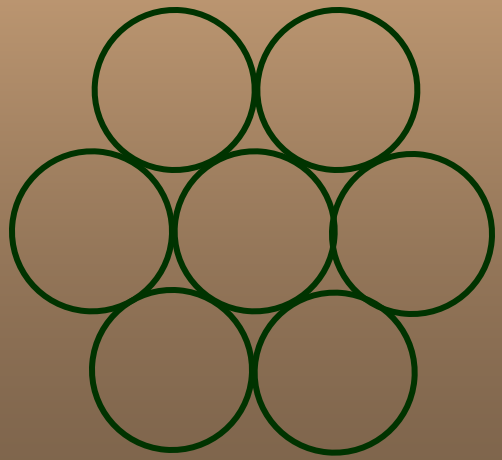


3. *Iron crystallizes in FCC lattice. The figures given below shows the iron atoms in four crystallographic planes.*

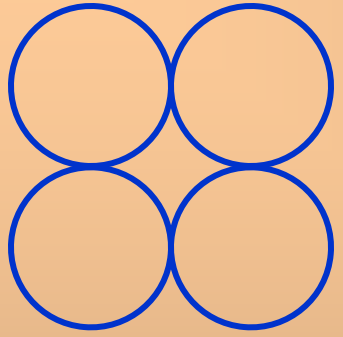


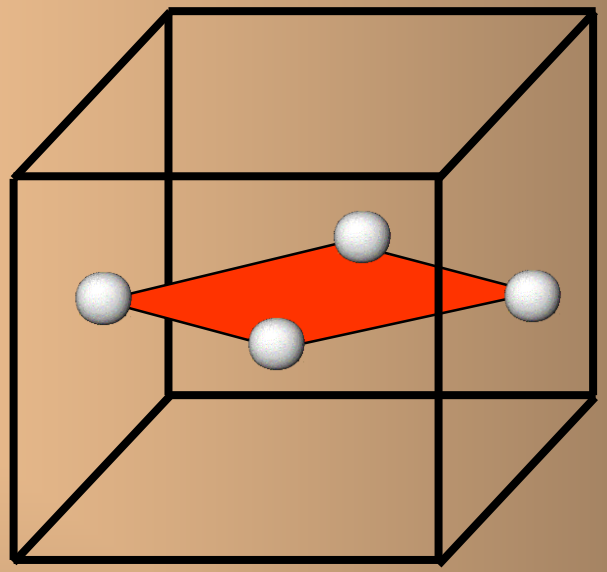




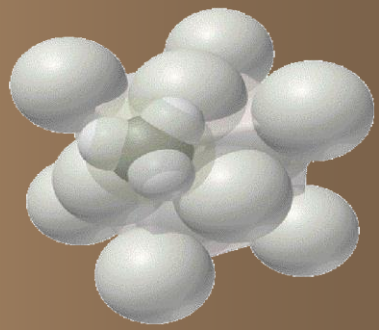


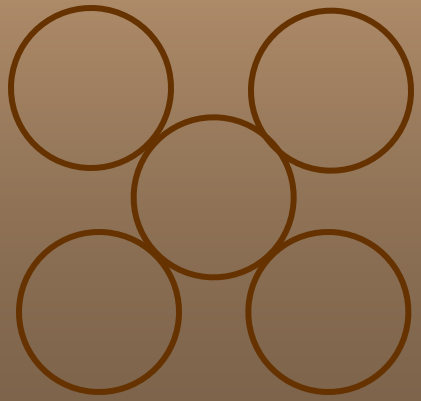
Draw the unit cell for the corresponding structure and identify these planes in the diagram. Also report the distance between two such crystallographic planes in each terms of the edge length 'a' of the unit cell.

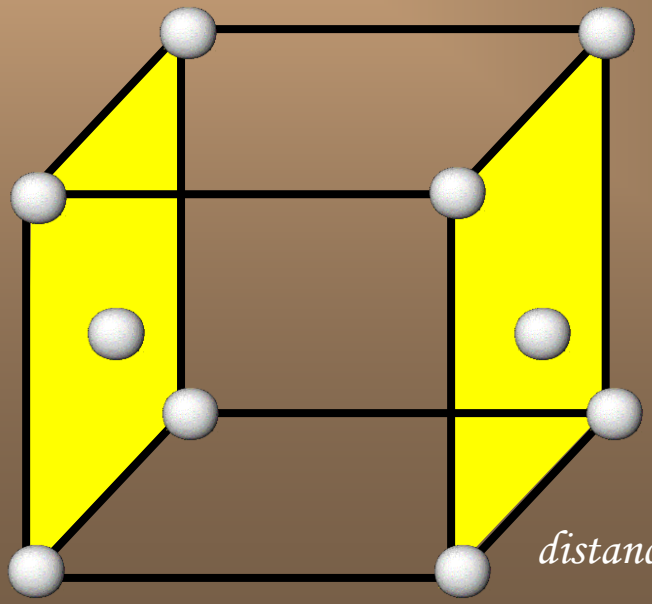




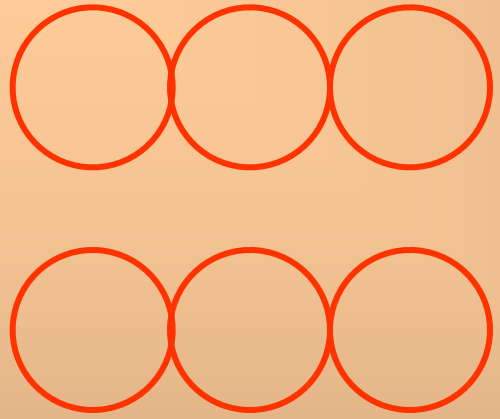
distance between two such planes is a

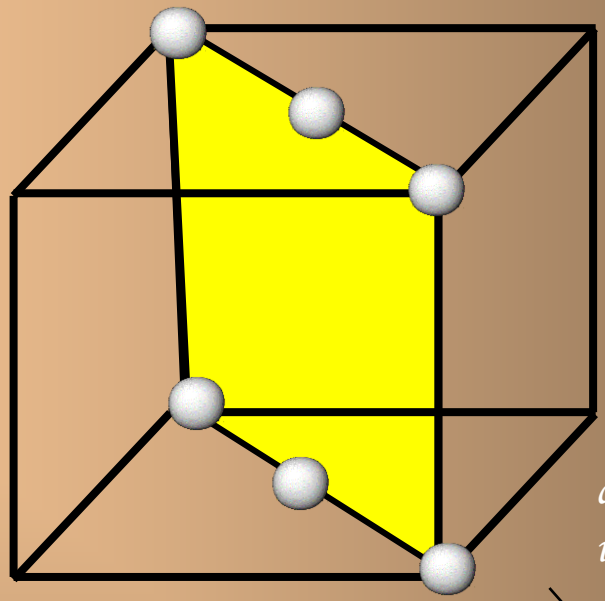


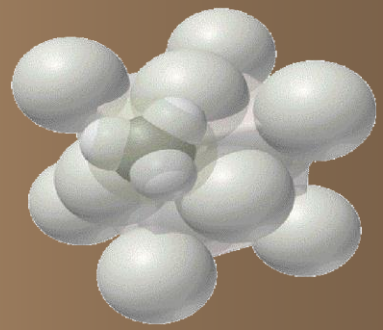




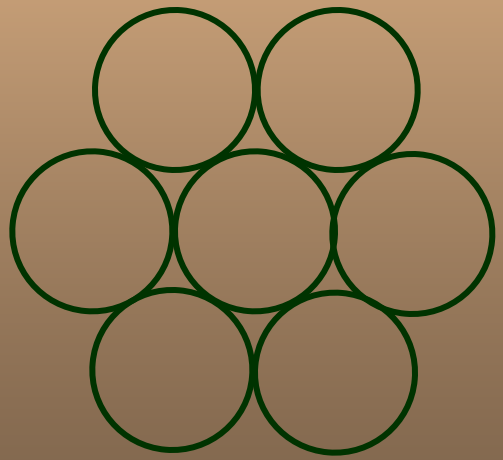
distance between two such planes is a

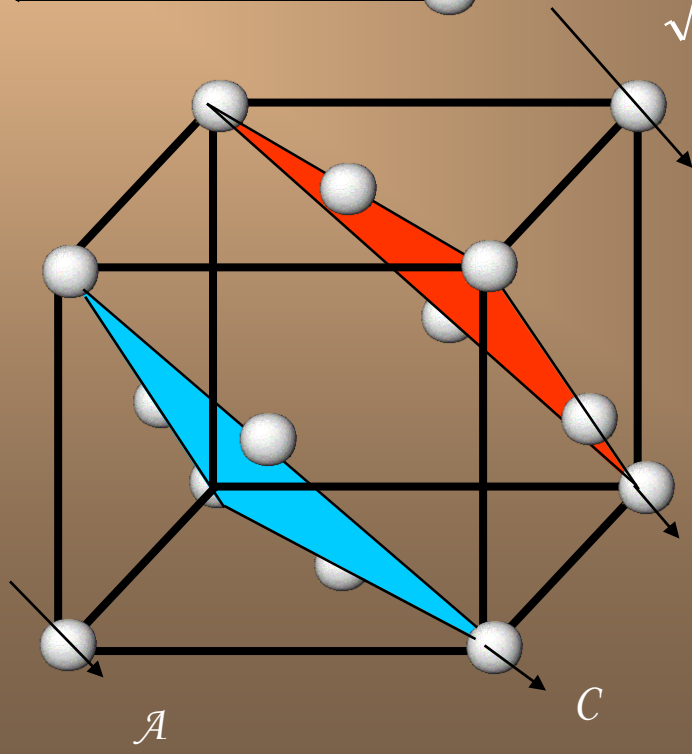






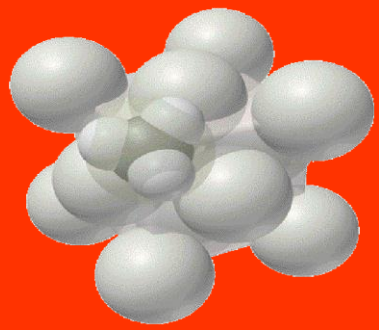
distance between two such planes is $\frac{a}{\sqrt{2}}$

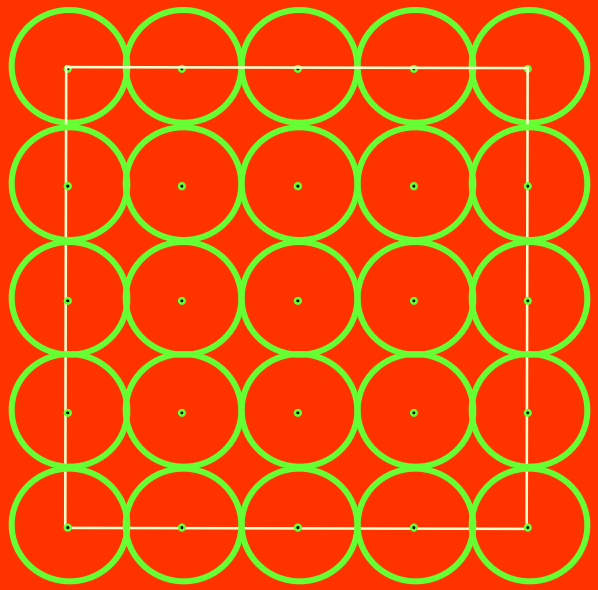




$$distance = \frac{\sqrt{3}a}{3} = \frac{a}{\sqrt{3}}$$

3. *Marbles of diameter 10 mm are to be placed on a flat surface bounded by lines of length 40 mm such that each marble has its centre within the bound surface. Find the maximum number of marbles in the bound surface and sketch the diagram. Derive an expression for the number of marbles per unit area.*



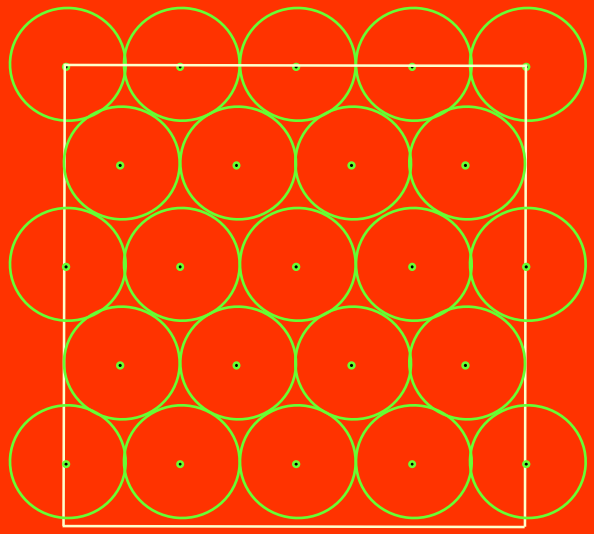


Interpretation:

1. count marbles as 1 each even if some portion goes outside the bound surface

2. count marbles based on the portion that is inside the bound surface

25



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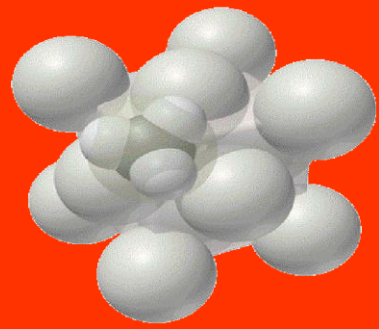

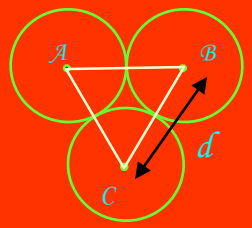

To calculate no. of marbles per unit area we need to select the smallest repeating unit.

$$\text{area of triangle } ABC = \frac{\sqrt{3}}{4}(d)^2$$

$$\text{no. of marbles in } \Delta ABC = 3 \times \frac{1}{6}$$

$$\text{no. of marbles per unit area} = \frac{1/2}{\sqrt{3}(10)^2/4} = 0.0115$$

based on this the total marbles in this enclosed figure $= 0.0115 \times 1600 = 18.4$