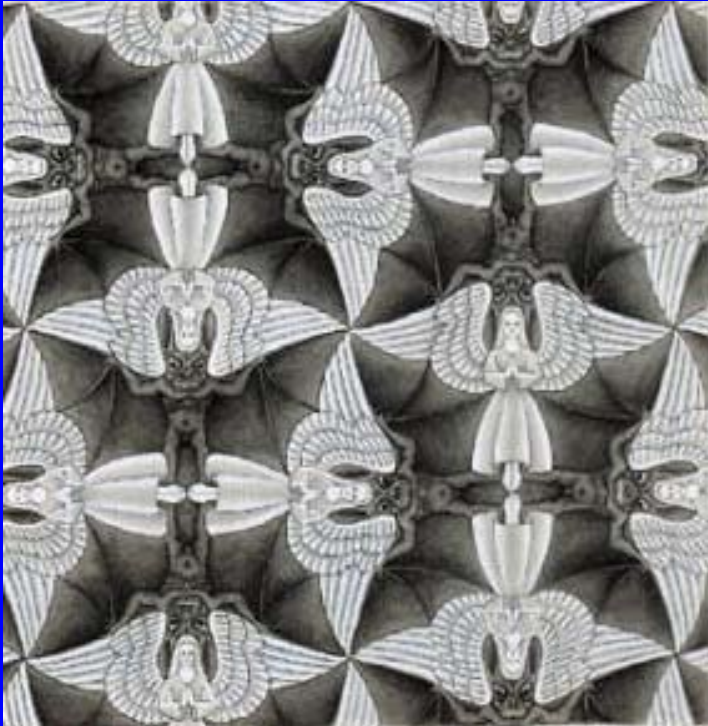
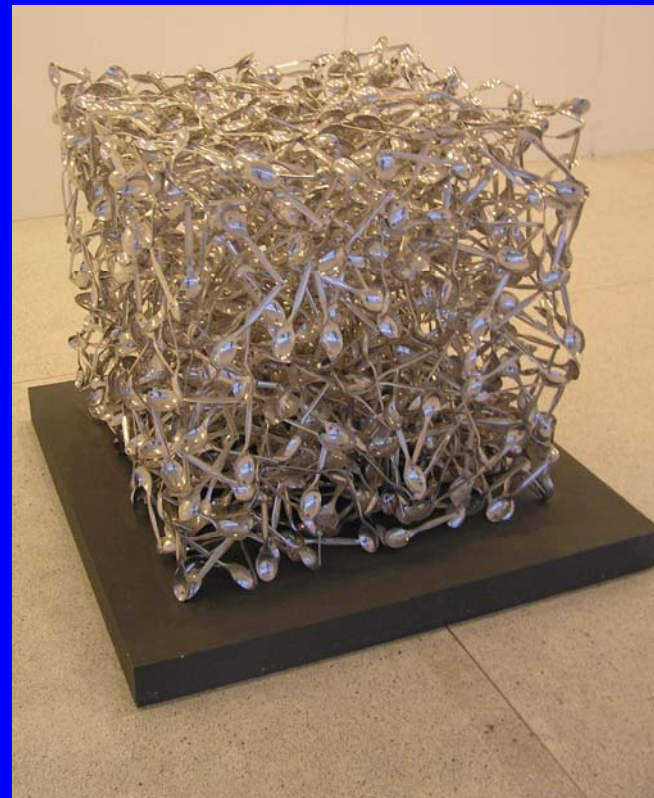


Struktura krystalických látek



Periodické opakování
stejných stavebních
jednotek



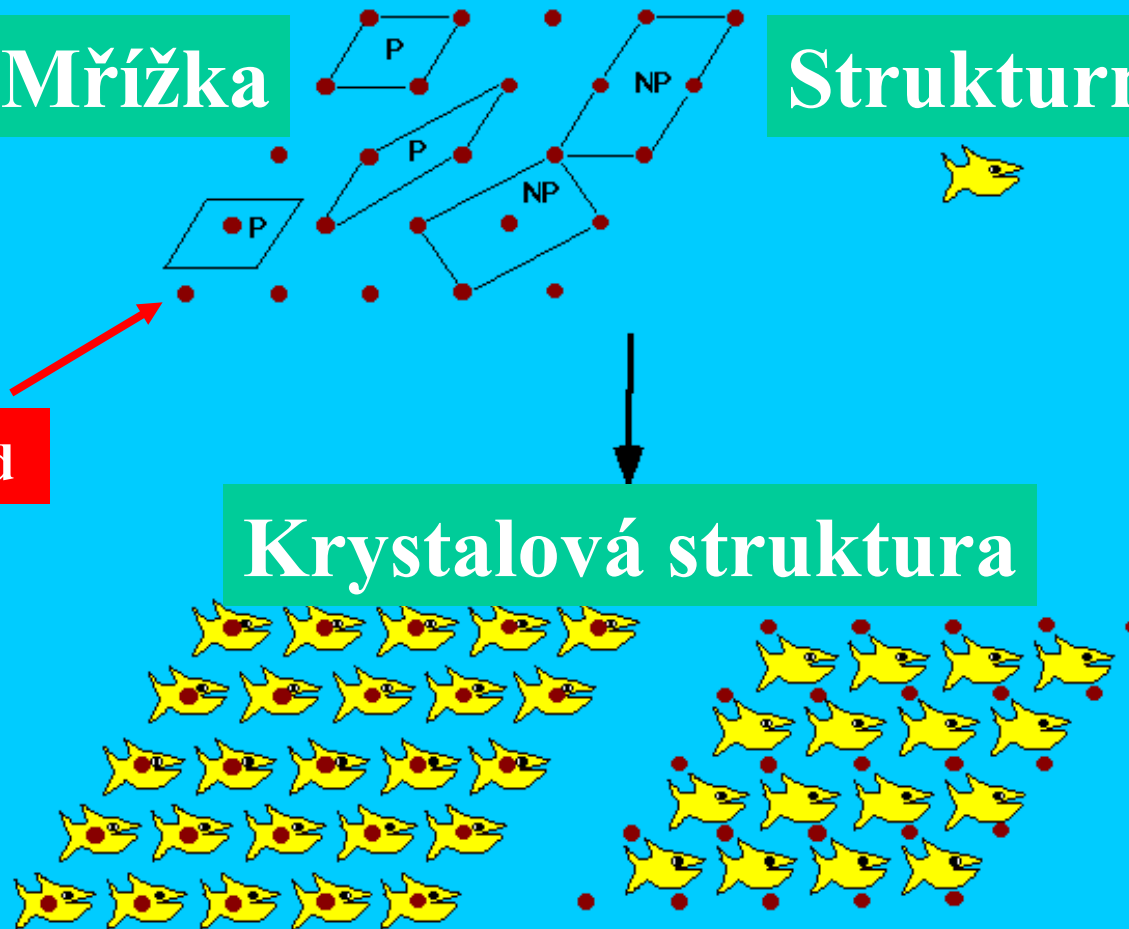
Mřížka a struktura

Mřížka

Strukturní motiv

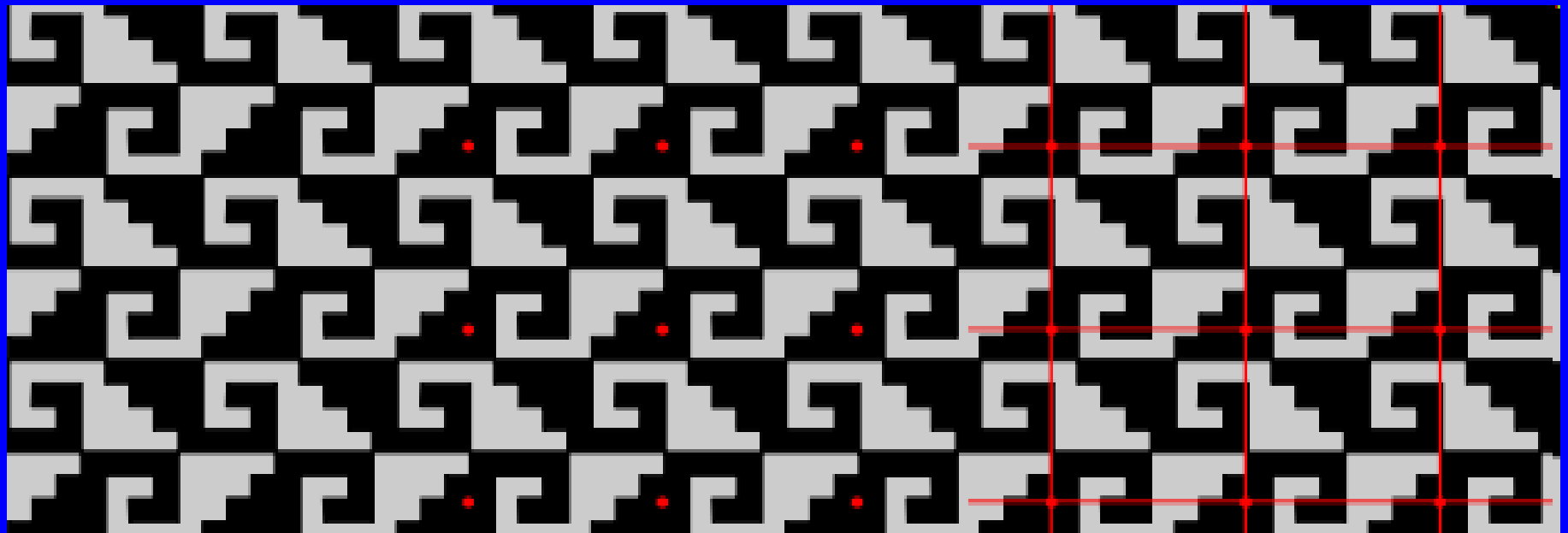
Uzlový bod

Krystalová struktura



Elementární buňka

Periodickým opakováním elementární buňky vytvoříme krystal

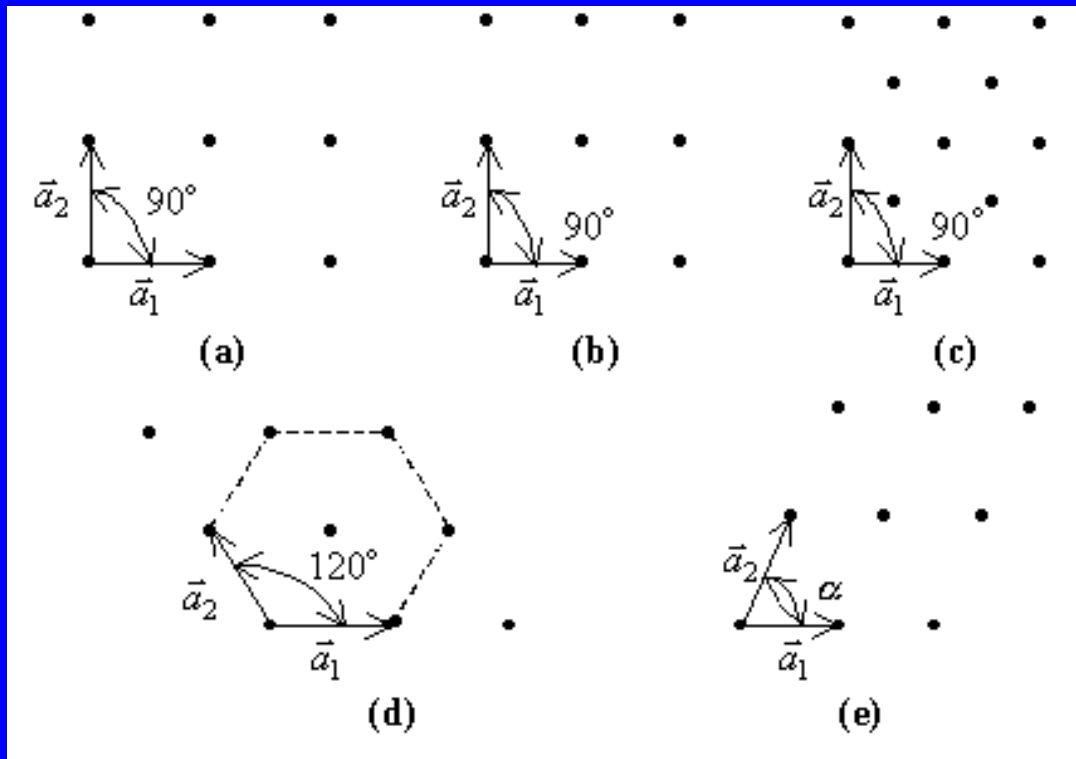


5 plošných mřížek

čtvercová

pravoúhlá

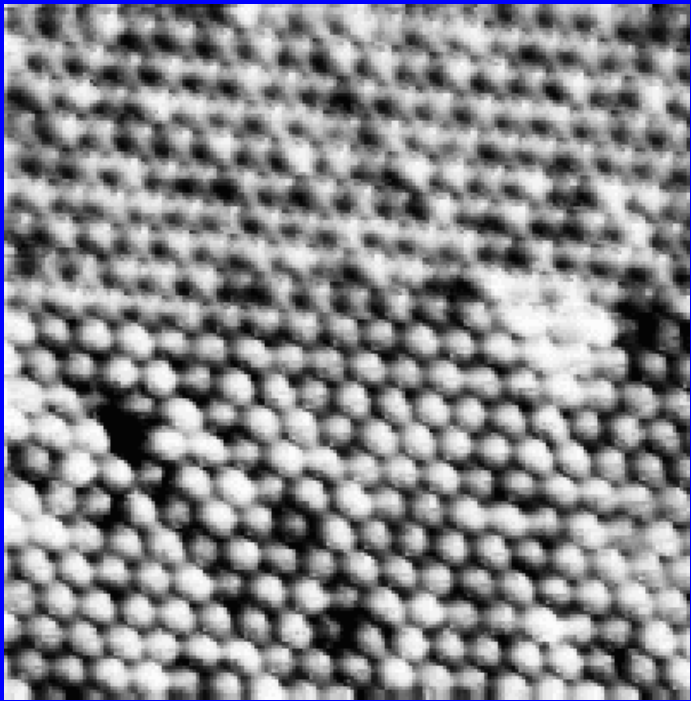
diamantová



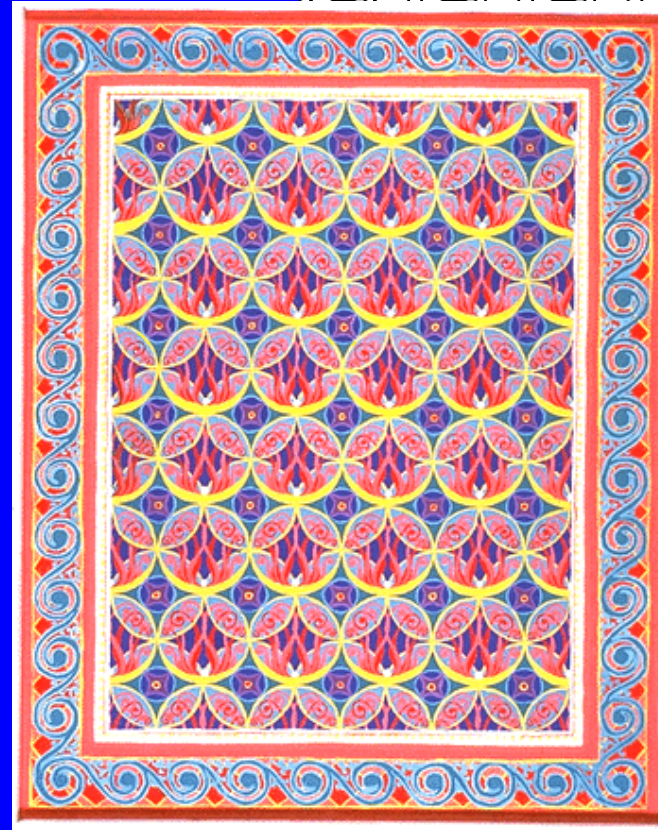
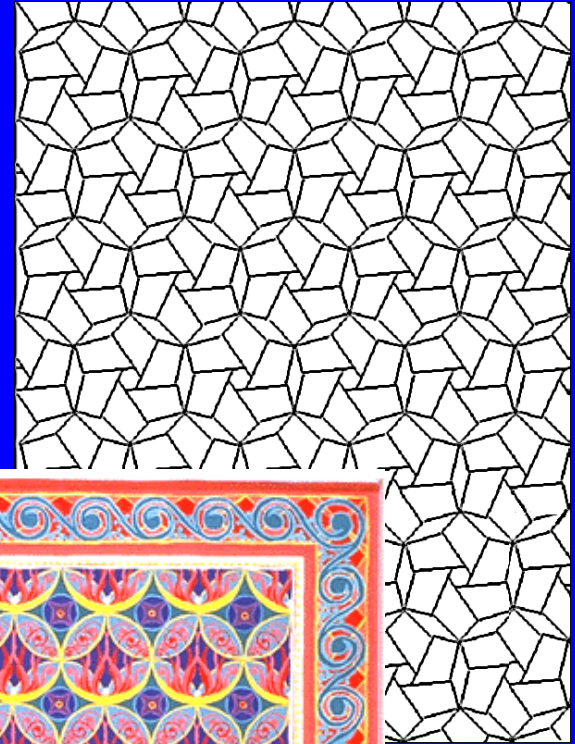
hexagonální

rovnoběžníková

Name	Number of Bravais lattices	Conditions
Square	1	$a_1 = a_2, \alpha = 90^\circ$
Rectangular	2	$a_1 \neq a_2, \alpha = 90^\circ$
Hexagonal	1	$a_1 = a_2, \alpha = 120^\circ$
Oblique	1	$a_1 \neq a_2, \alpha \neq 120^\circ, \alpha \neq 90^\circ$



STM Nb/Se

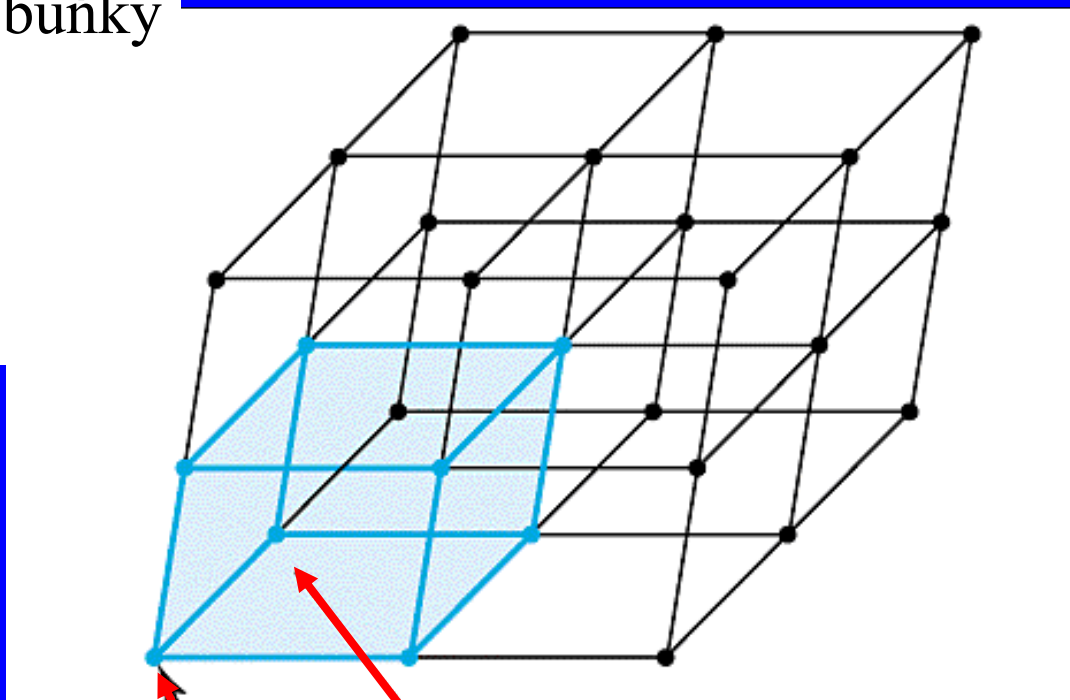


Mřížka a elementární buňka

Parametry elementární buňky

a, b, c – délky hran

α, β, γ – velikosti úhlů



Uzlový bod

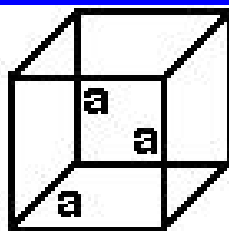
Elementární buňka

Sedm krystalových systémů

Krychlová
kubická

$$a = b = c$$

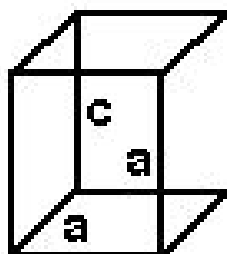
$$\alpha = \beta = \gamma = 90^\circ$$



Čtverečná
tetragonální

$$a = b \neq c$$

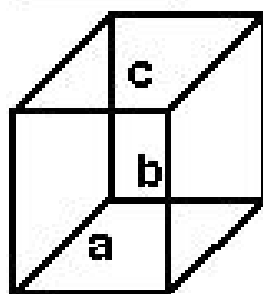
$$\alpha = \beta = \gamma = 90^\circ$$



Kosočtverečná
ortorombická

$$a \neq b \neq c$$

$$\alpha = \beta = \gamma = 90^\circ$$



Trigonální
romboedrická

$$a = b = c$$

$$\alpha = \beta = \gamma \neq 90^\circ$$

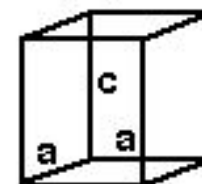


Šesterečná
hexagonální

$$a = b \neq c$$

$$\alpha = \beta = 90^\circ$$

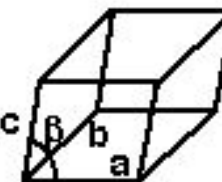
$$\gamma = 120^\circ$$



Jednoklonná
monoklinická

$$a \neq b \neq c$$

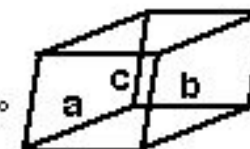
$$\alpha = \gamma = 90^\circ \neq \beta$$













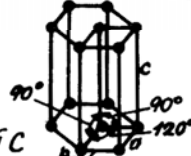



Trojklonná
triklinická

$$a \neq b \neq c$$

$$\alpha \neq \beta \neq \gamma \neq 90^\circ$$

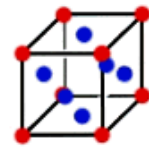


14 Bravaisových mřížek

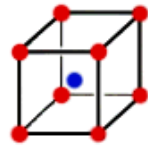
Krystalová soustava	Čtrnáct Bravaisových mříží s osami a úhly jednotkových buněk
trojklonná (triklinická)	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90^\circ$  P (jednoduchá)
jednoklonná (monoklinická)	$a \neq b \neq c$ $\alpha = \gamma = 90^\circ \neq \beta$  P (jednoduchá)  C (basálně centrovaná)
kosočtverečná (ortorombická)	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$ I (prostorově) F (plošně)  P (jednoduchá)  C (basálně centr.)  I (prostorově)  F (plošně) centrovaná)
trigonální (romboedrická)	$a = b = c$ $\alpha = \beta = \gamma < 120^\circ, 90^\circ$  trigonální R
čtverečná (tetragonální)	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$  P (jednoduchá)  I (prostorově) centrovaná)
šesterečná (hexagonální)	$a = b \neq c$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$  šesterečná C a trigonální C
krychlová (kubická)	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$ I (prostorově) F (plošně)  P (jednoduchá)  I (prostorově) centrovaná)  F (plošně)



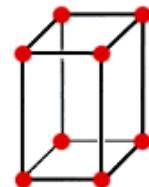
Simple cubic



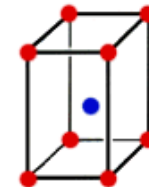
Face-centered cubic



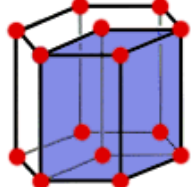
Body-centered cubic



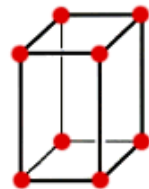
Simple tetragonal



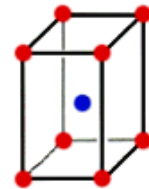
Body-centered tetragonal



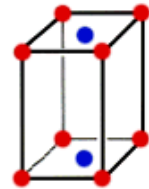
Hexagonal



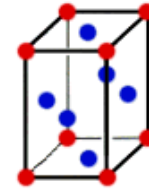
Simple orthorhombic



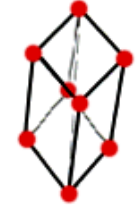
Body-centered orthorhombic



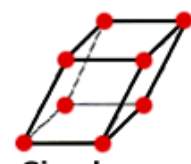
Base-centered orthorhombic



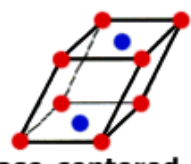
Face-centered orthorhombic



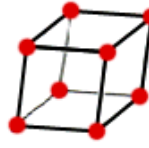
Rhombohedral



Simple Monoclinic



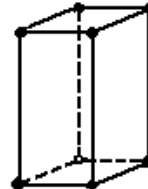
Base-centered monoclinic



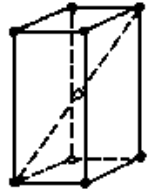
Triclinic



aP
triklinická

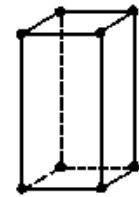


mP

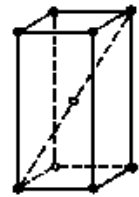


mI

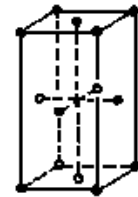
monolinická



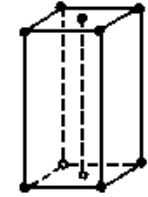
oP



oI

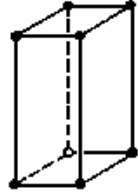


oF

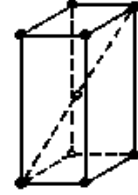


oC

ortorombická

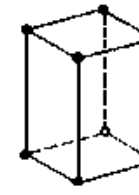


tP

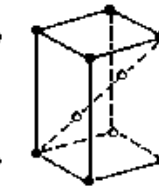


tI

tetragonální

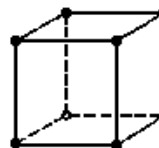


hP

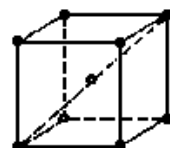


hR

hexagonální

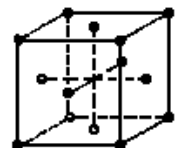


cP



cI

kubická

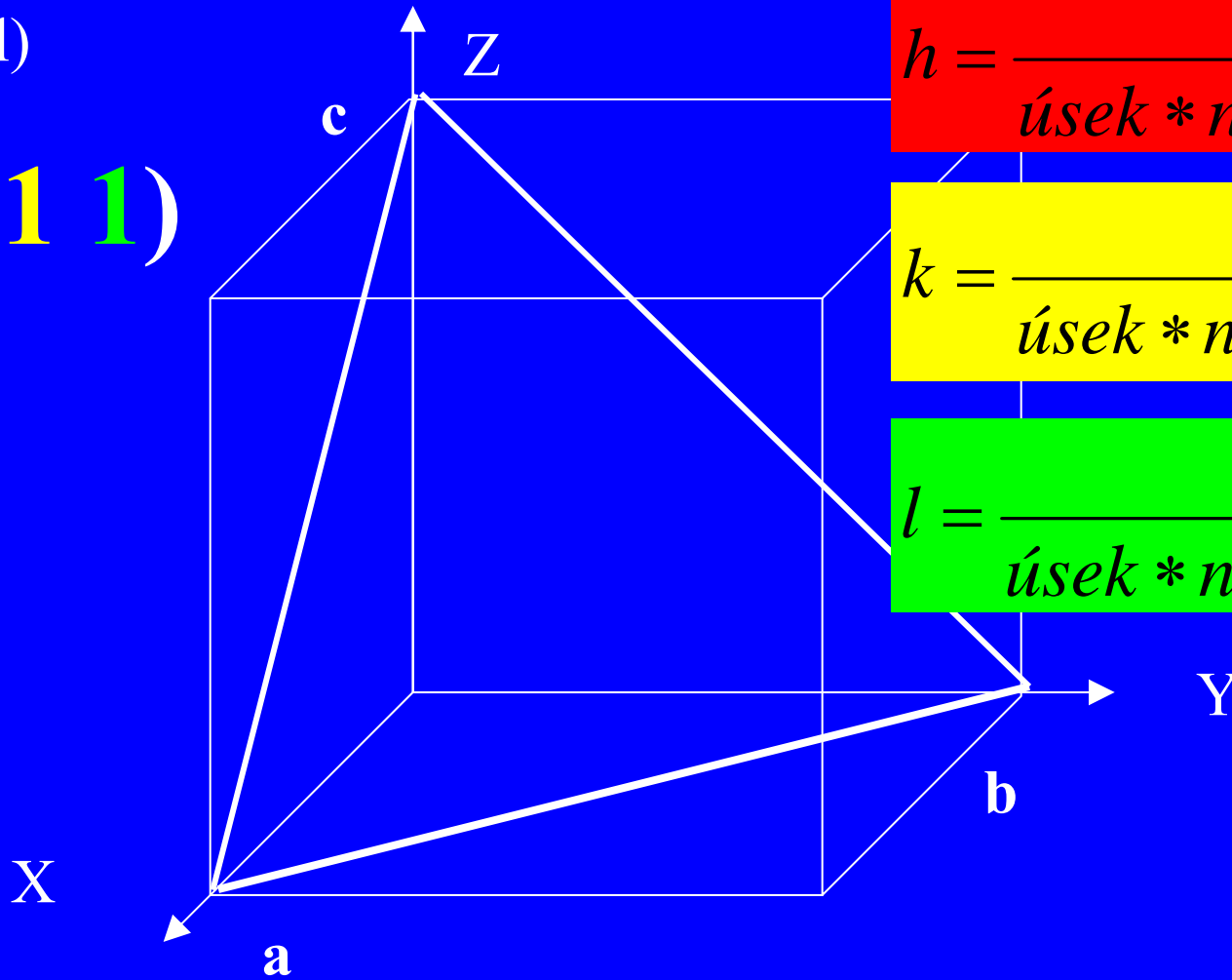


cF

Millerovy indexy

(h k l)

(1 1 1)

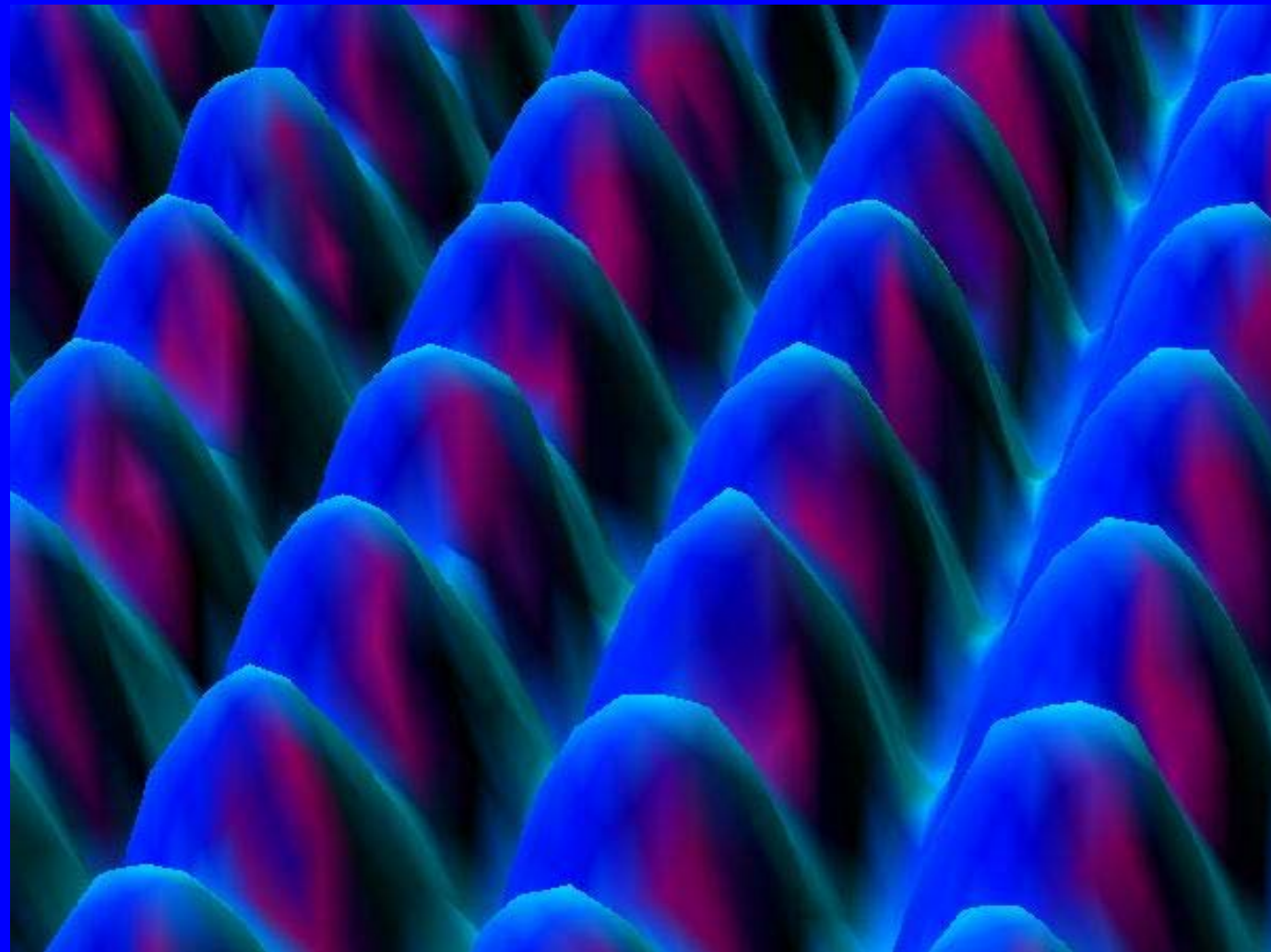


$$h = \frac{1}{\text{úsek} * na * ose * x}$$

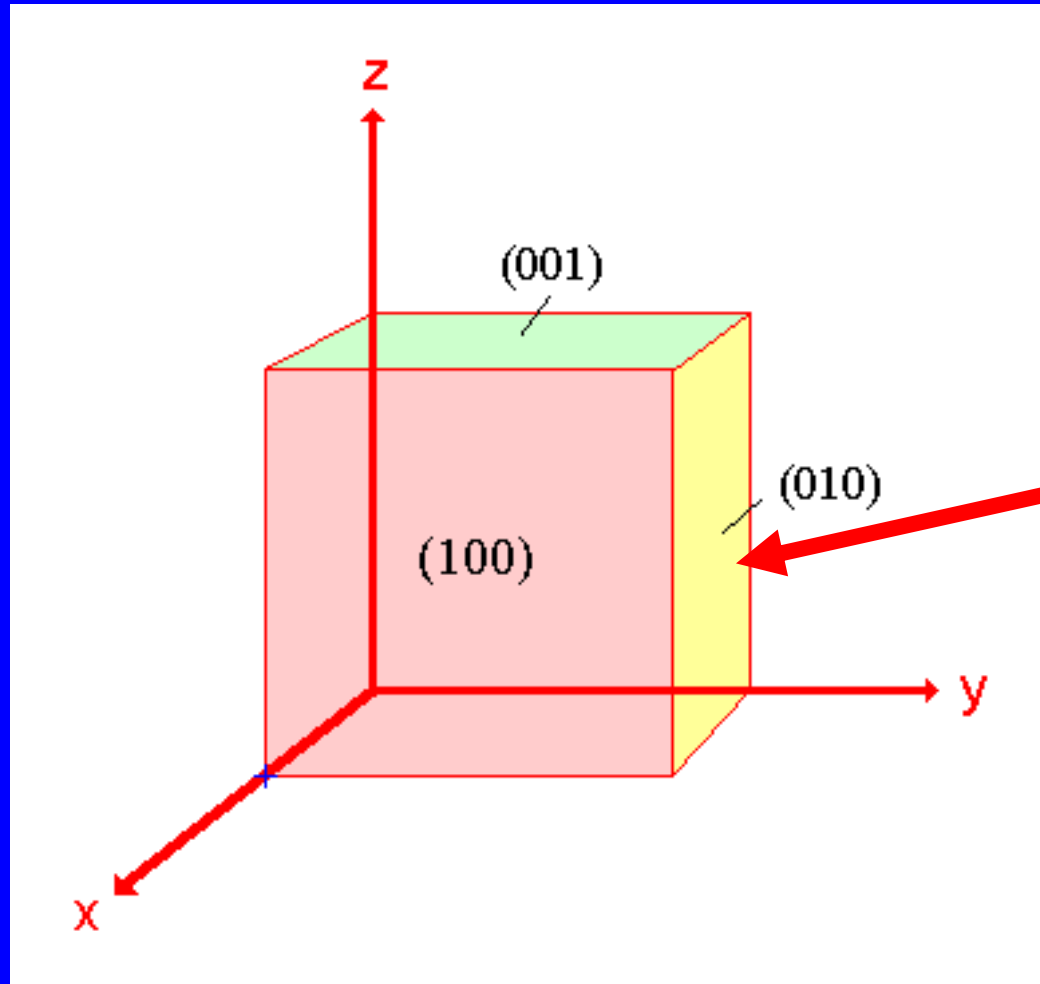
$$k = \frac{1}{\text{úsek} * na * ose * y}$$

$$l = \frac{1}{\text{úsek} * na * ose * z}$$

STM obraz Fe v (110) rovině



Millerovy indexy

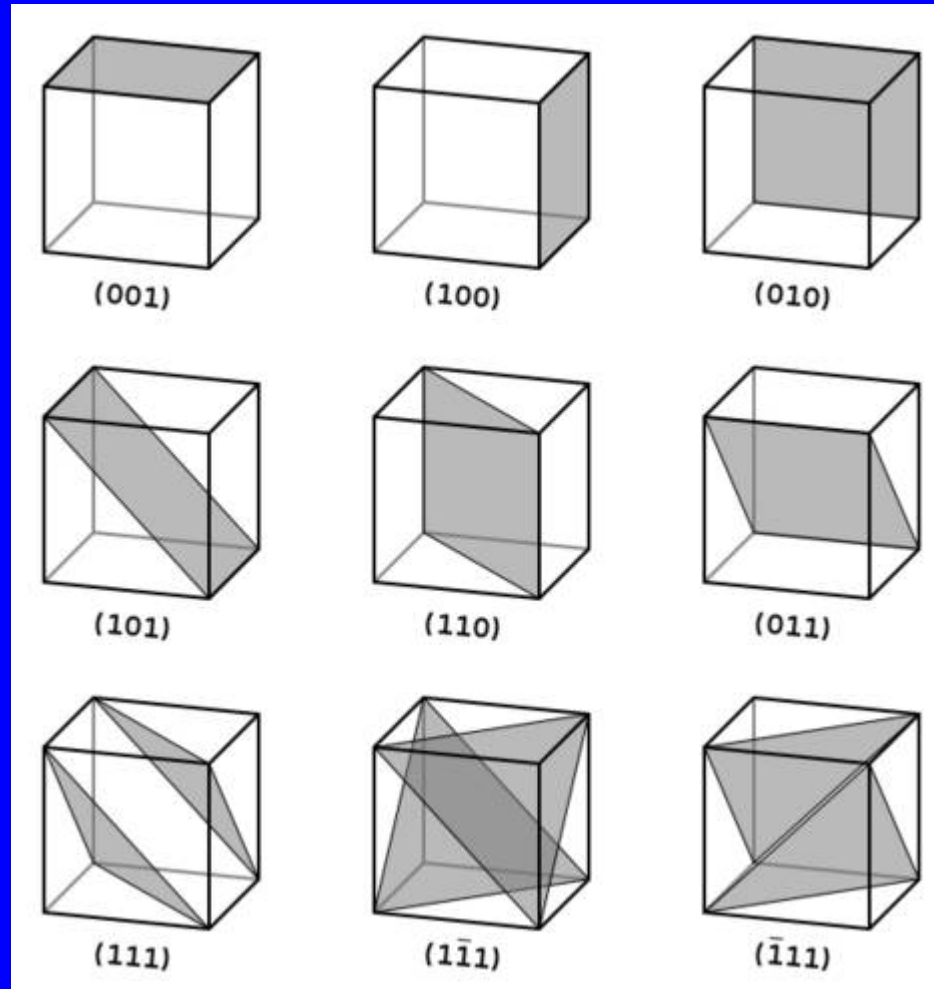


$h = 1/\text{úsek na } x$
 $k = 1/\text{úsek na } y$
 $l = 1/\text{úsek na } z$

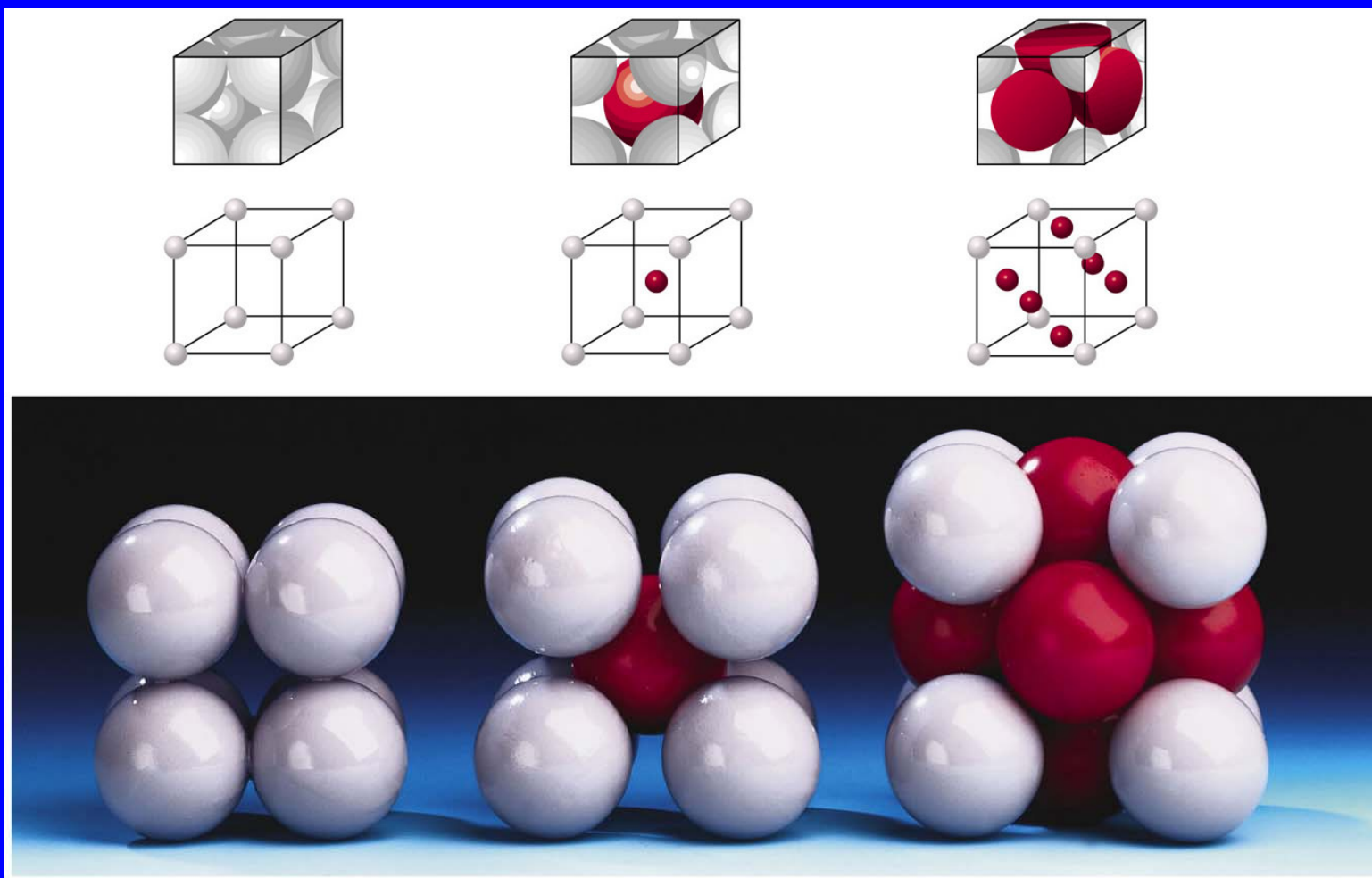
$(0\ 1\ 0)$

$h = 1 / \infty = 0$
 $k = 1 / 1 = 1$
 $l = 1 / \infty = 0$

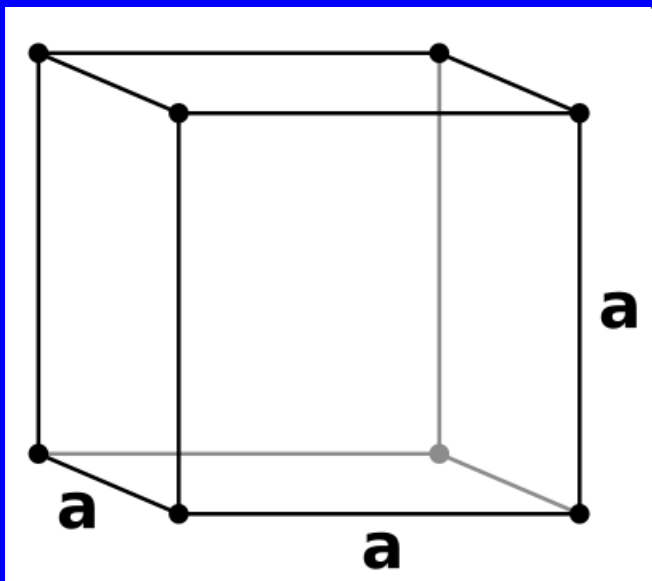
Millerovy indexy



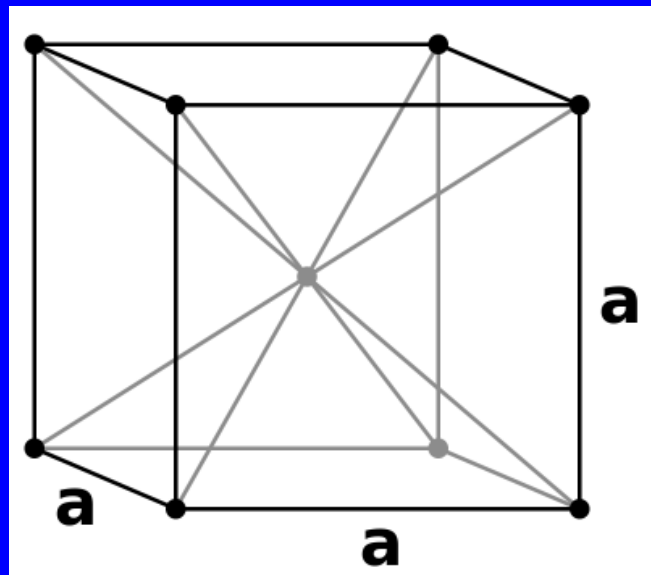
3 kubické buňky



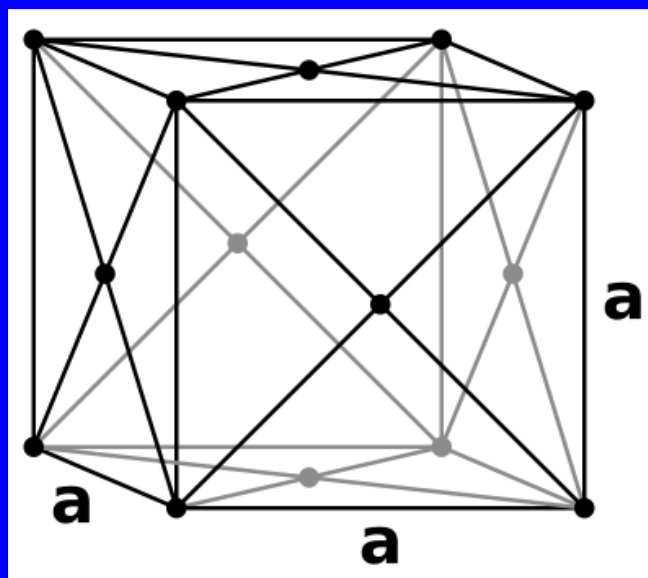
Primitivní (P) Prostorově centrovaná (I) Plošně centrovaná (F)



Primitivní (P)



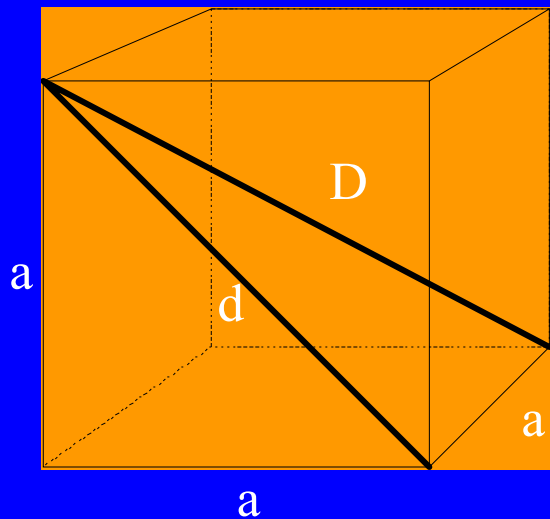
Prostorově centrovaná (I)



Plošně centrovaná (F)

Krychle

a = hrana



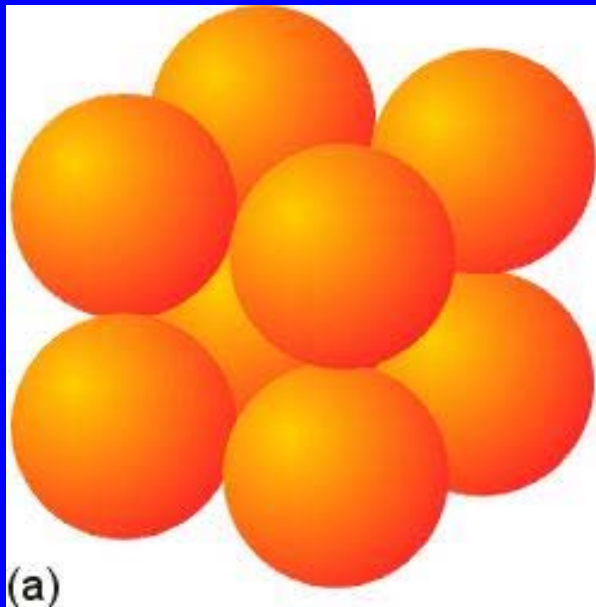
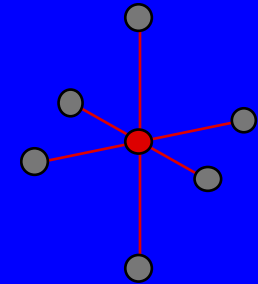
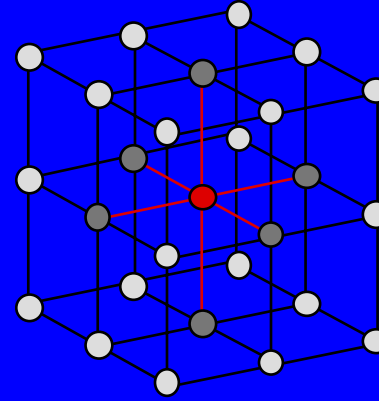
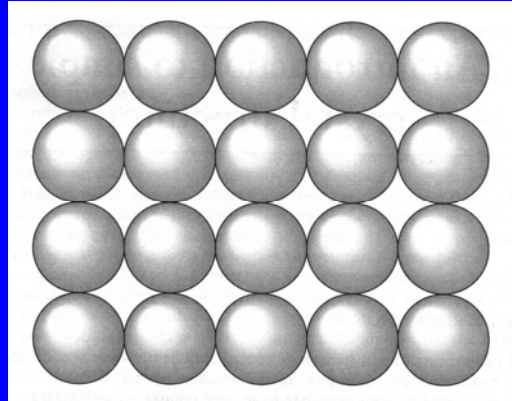
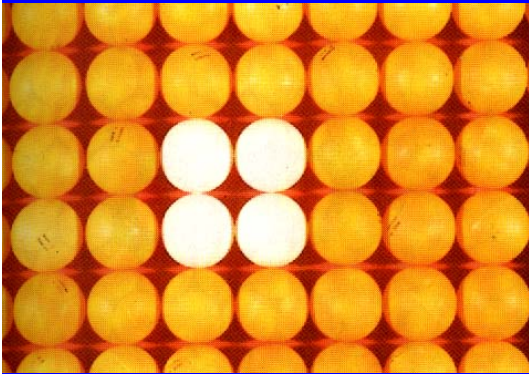
d = stěnová diagonála
($d^2 = a^2 + a^2 = 2a^2$)

D = tělesová diagonála
($D^2 = d^2 + a^2 = 2a^2 + a^2 = 3a^2$)

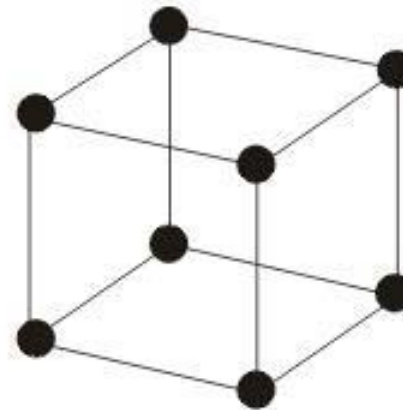
$$d = \sqrt{2} \cdot a$$

$$D = \sqrt{3} \cdot a$$

Primitivní kubická buňka, Po - Litviněnko



(a)



(b)

Zaplnění prostoru
52%

Koord. číslo 6

Primitivní kubická buňka

Počet uzlových bodů v buňce

$$\frac{1/8 \text{ atomu}}{\text{vrchol}} \times 8 \text{ vrcholů} = \frac{1 \text{ atom}}{\text{buňku}}$$

Zaplnění prostoru

atomy se dotýkají podél hrany (a)

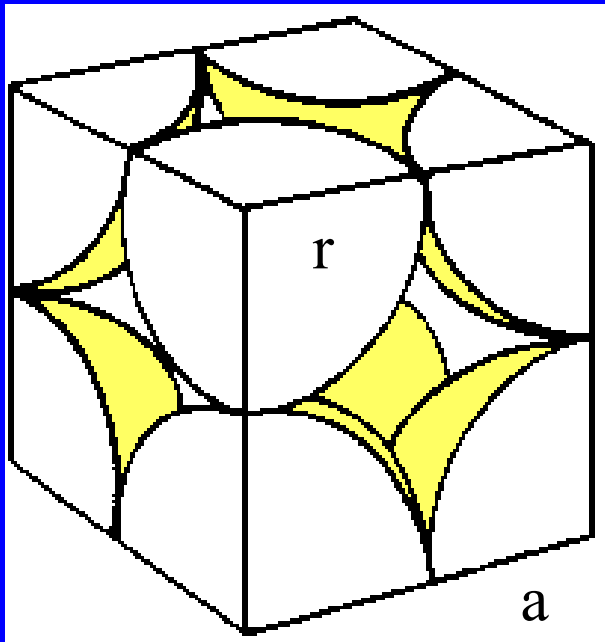
$$a = 2r \quad \text{potom} \quad r = \frac{a}{2}$$

$$\text{Objem buňky } V = a^3 = 8r^3$$

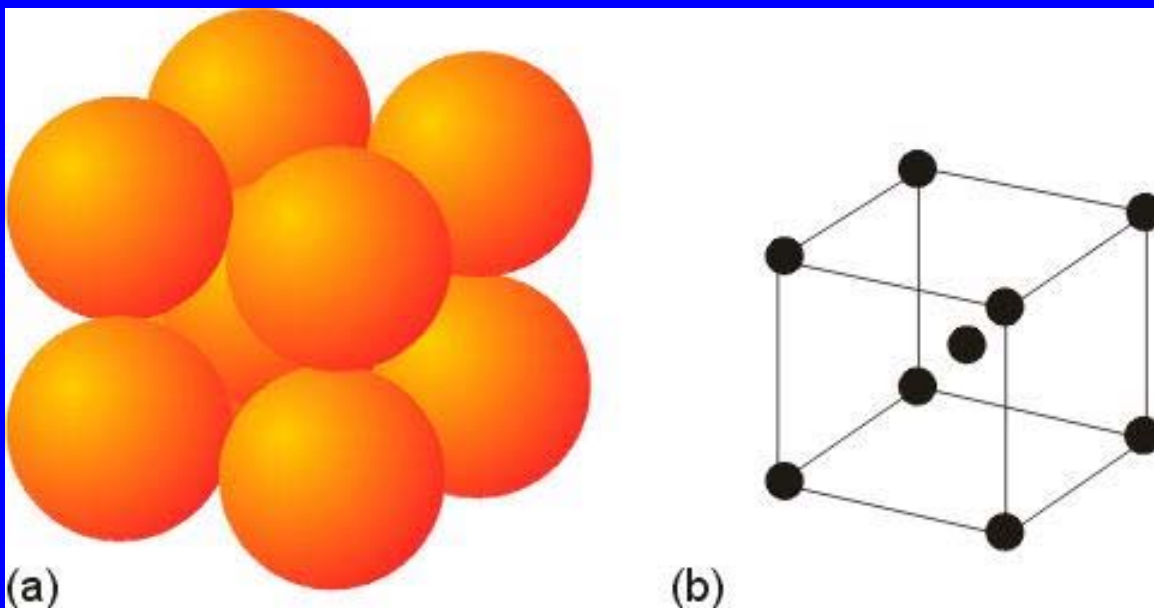
Objem atomu uvnitř buňky

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

$$\text{Procento zaplnění} = \frac{V_A}{V} 100 = 52\%$$



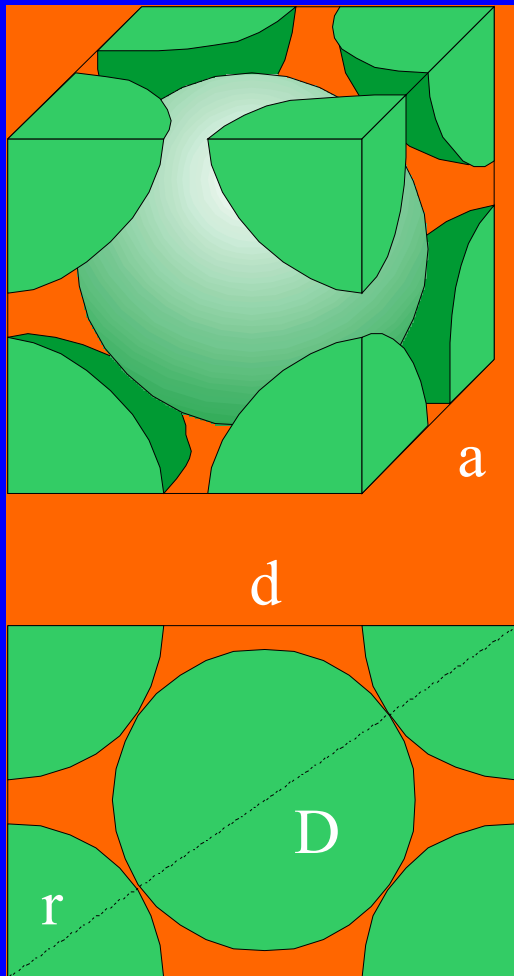
Tělesně centrovaná buňka, W



Zaplnění prostoru 68%

Koord. číslo 8

Tělesně centrovaná buňka, W



Počet atomů v buňce

$$\frac{1/8 \text{ atomu}}{\text{vrchol}} \times 8 \text{ vrcholů} = 1 \text{ atom}$$
$$+ \text{střed} = 1 \text{ atom}$$
$$\underline{\underline{2 \text{ atomy/buňku}}}$$

atomy se dotýkají podél tělesové diagonály (D)

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

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

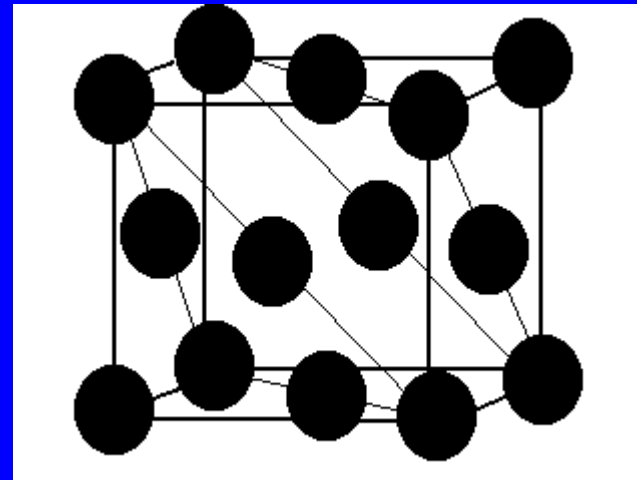
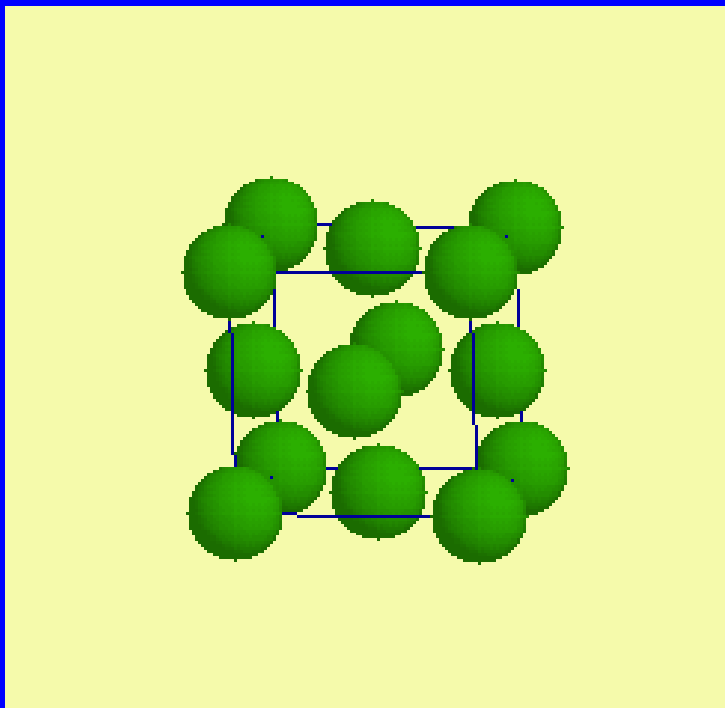
potom

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

$$V = a^3 = \left(\frac{4r}{\sqrt{3}} \right)^3$$



Plošně centrovaná buňka, Cu (= nejtěsnější kubické uspořádání)



Zaplnění prostoru 74%

Koord. číslo 12

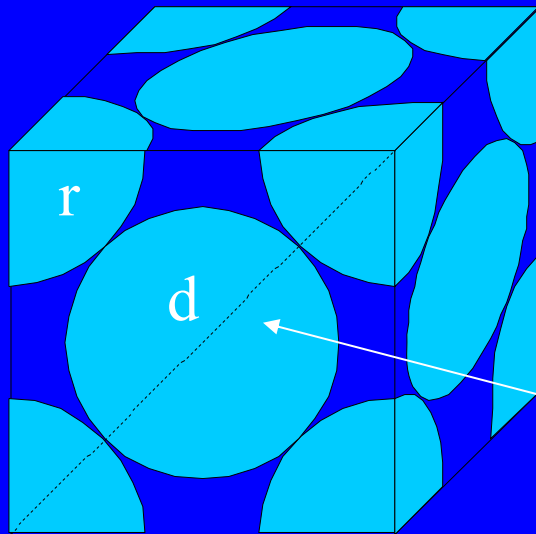
Plošně centrovaná buňka

Počet atomů v buňce

$$\frac{1/8 \text{ atomu}}{\text{vrchol}} \times 8 \text{ vrcholů} = 1 \text{ atom}$$

$$\frac{1/2 \text{ atomu}}{\text{stěnu}} \times 6 \text{ stěn} = 3 \text{ atomy}$$

4 atomy/buňku



atomy se dotýkají podél stěnové diagonály (d)

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

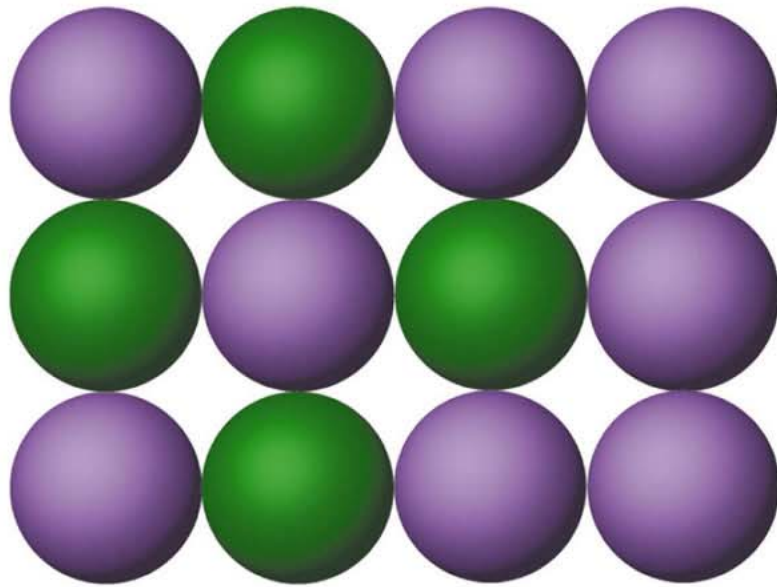
$$a = \frac{4r}{\sqrt{2}} \quad \text{or} \quad r = \frac{\sqrt{2} \cdot a}{4}$$

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

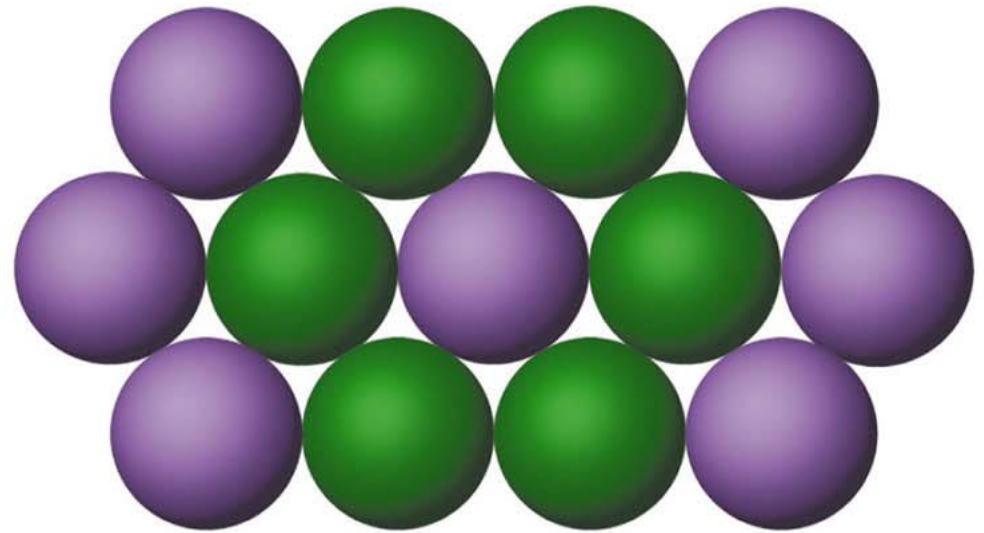
Zaplnění prostoru

	Poloměr	Počet atomů	Zaplnění
Primitivní kubická	$a/2$	1	52%
Tělesně centrovaná	$\sqrt{3}a/4$	2	68%
Plošně centrovaná	$\sqrt{2}a/4$	4	74%
Diamant	$\sqrt{3}a/8$	8	34%

Nejtěsnější uspořádání na ploše



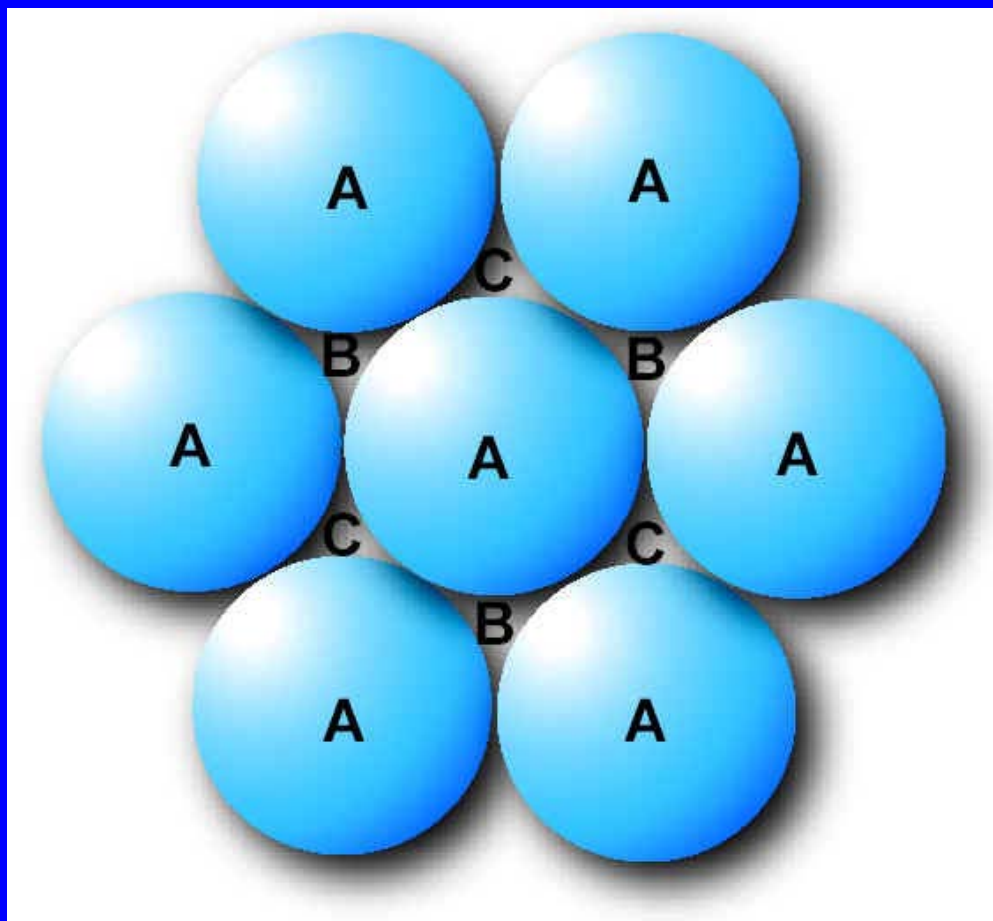
(a) An "open" packing



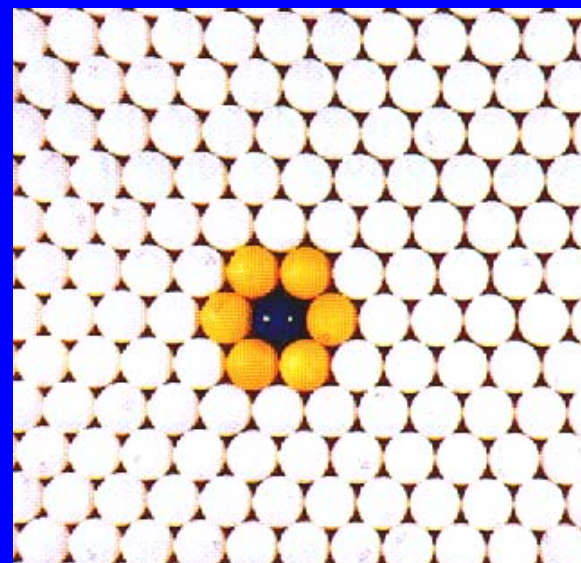
(b) Close packing

Čtvercové uspořádání
Hodně volného prostoru
4 sousední atomy

Hexagonální uspořádání
Nejlepší využití prostoru
6 sousedních atomů



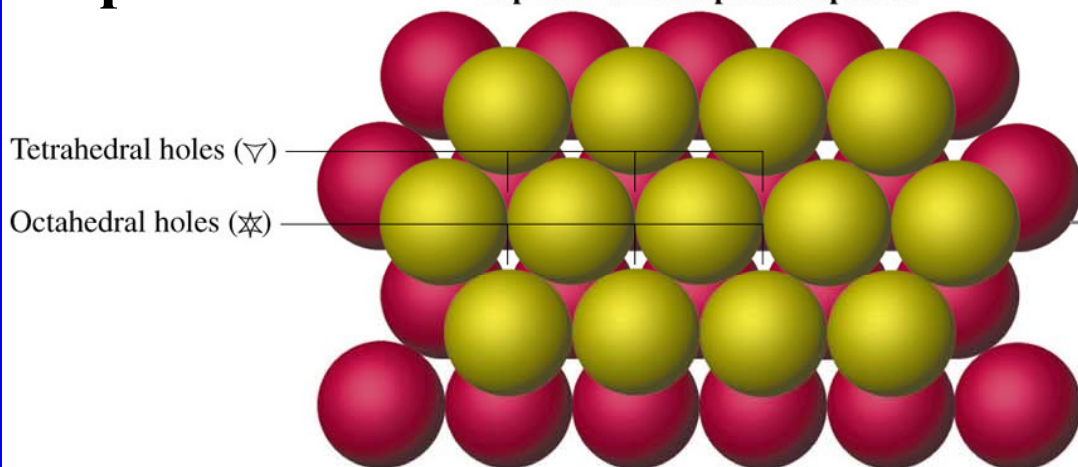
Mezery B a C nemohou být zároveň obsazeny atomy (v druhé vrstvě)



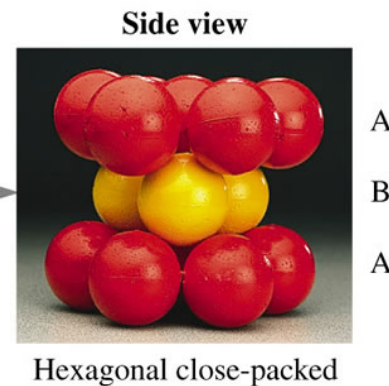
Dvě vrstvy nejtěsnějšího uspořádání

hexagonální

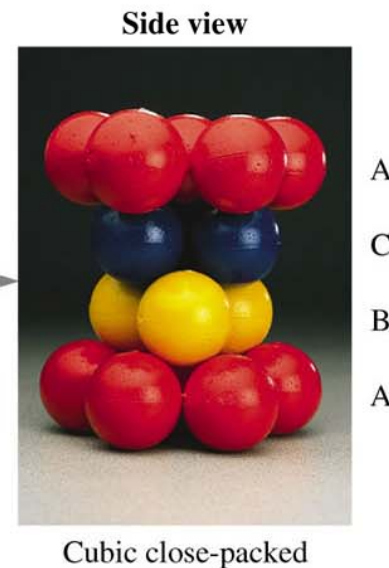
Top view of close-packed spheres



Cover tetrahedral holes in layer B



Cover octahedral holes in layer B

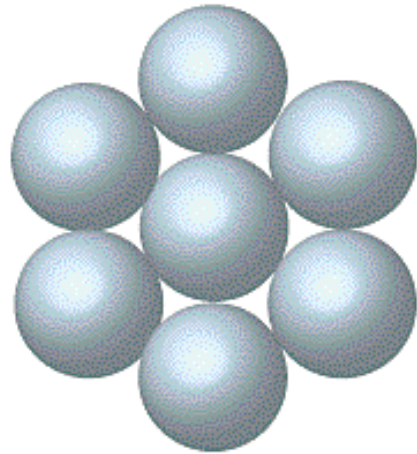


kubické

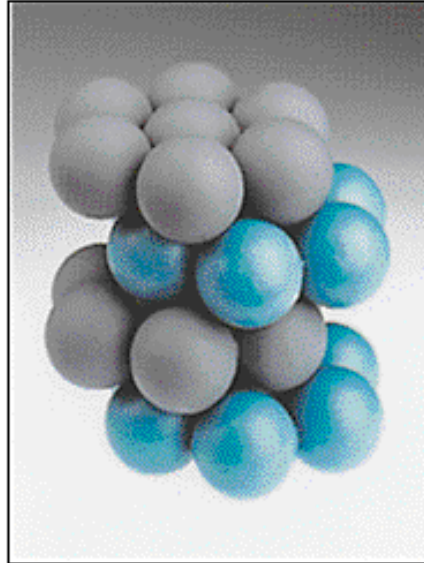


Johannes Kepler 1611

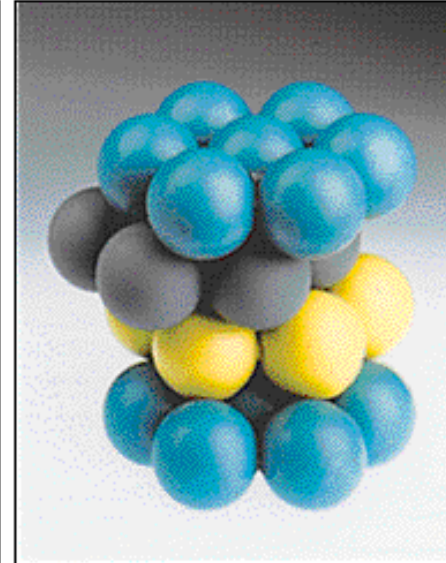
Nejtěsnější uspořádání v prostoru



Close-packed layer of spheres



(b)



(c)

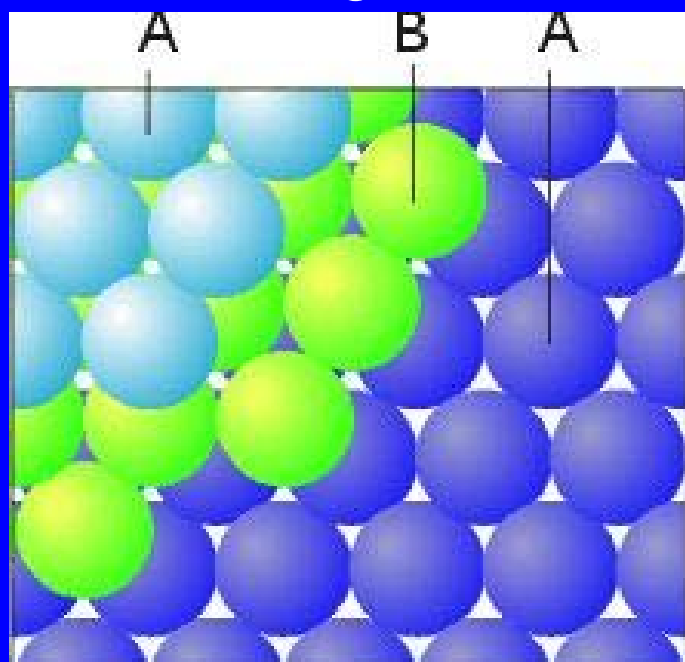


Johannes Kepler 1611

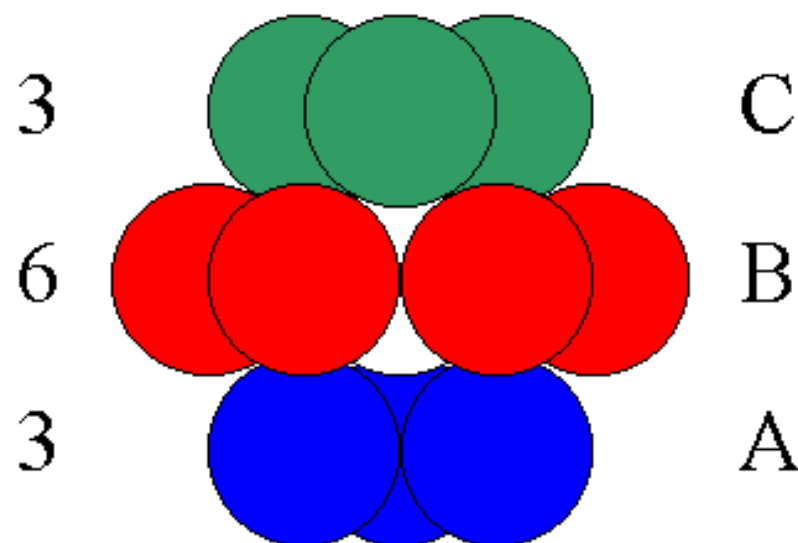
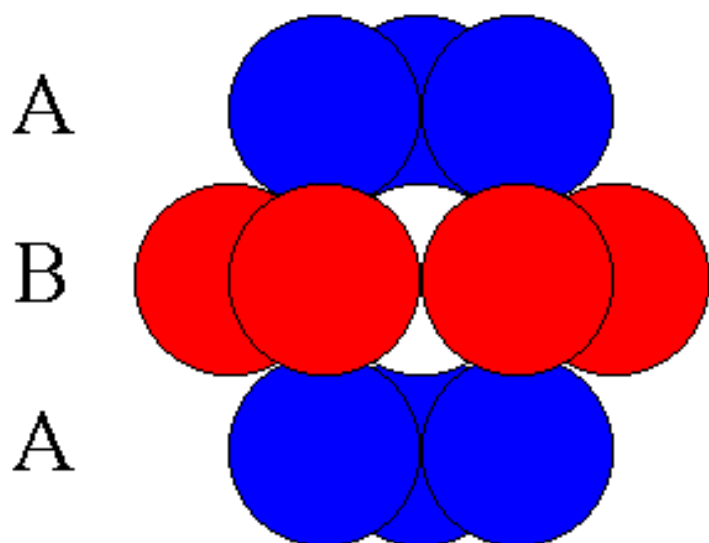
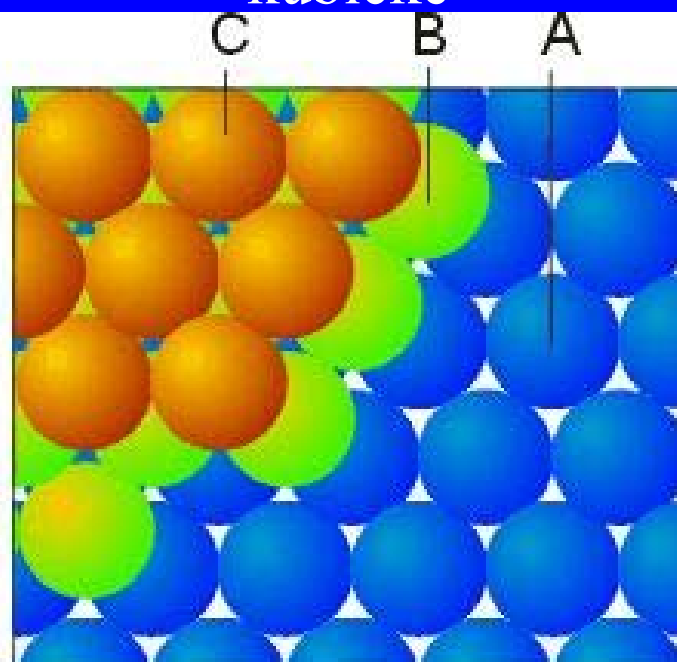
hexagonální

kubické

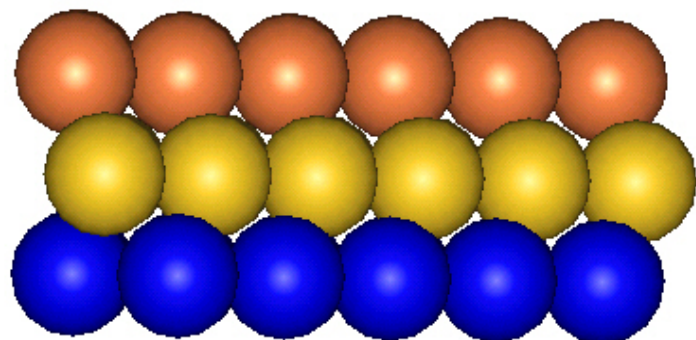
hexagonální



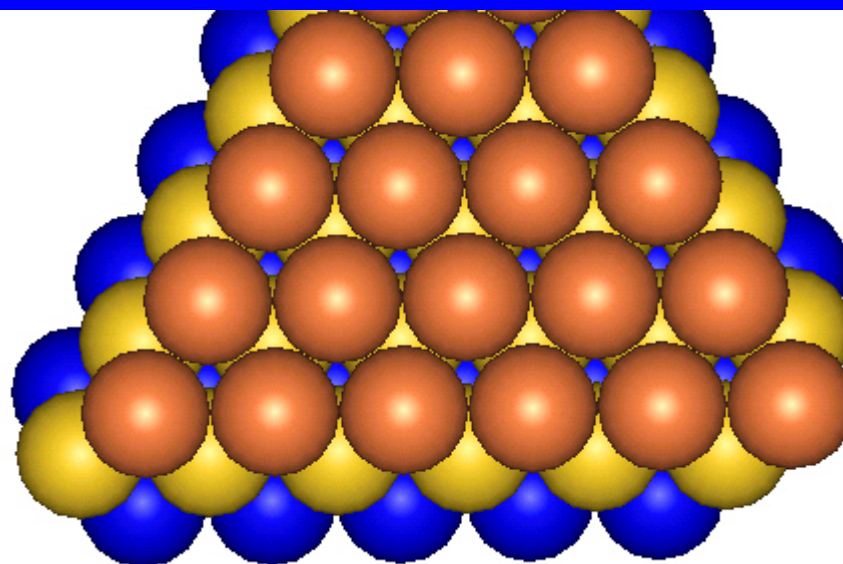
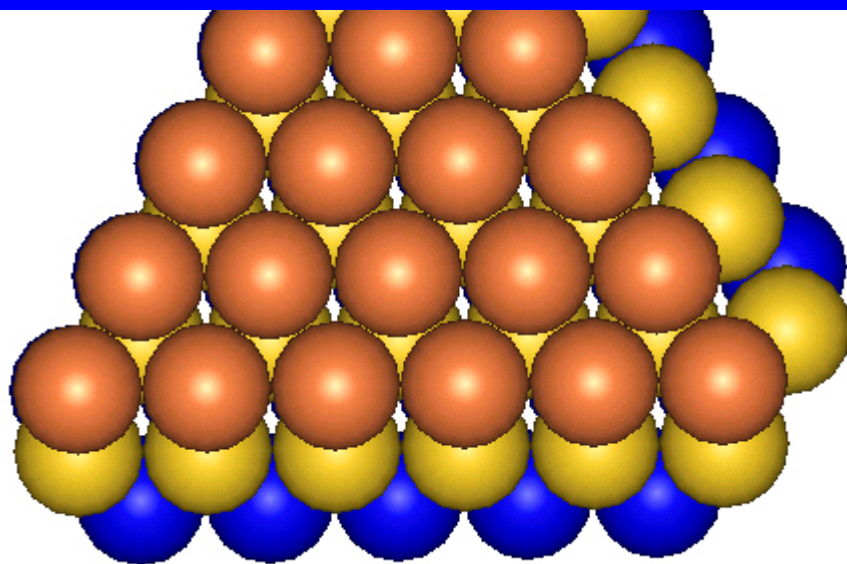
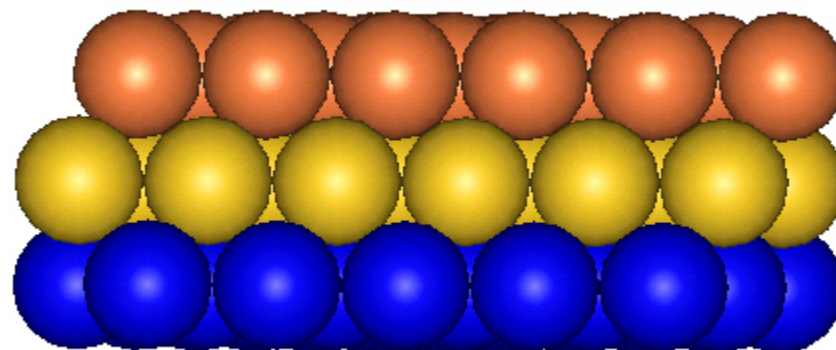
kubické



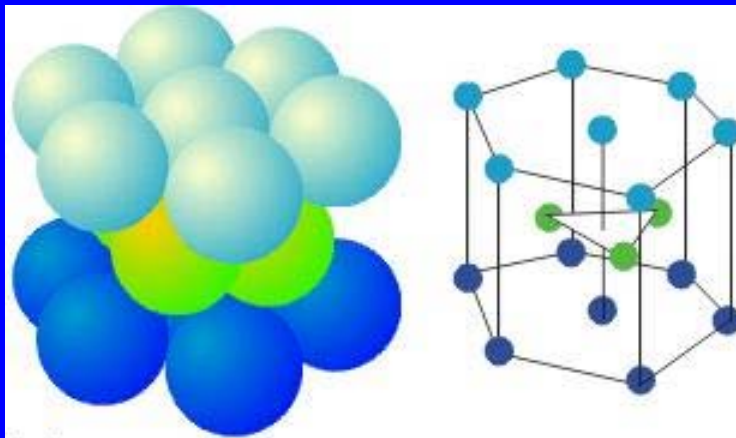
hexagonální



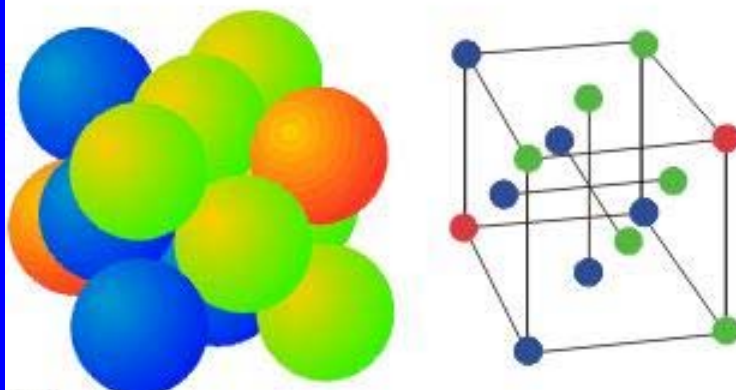
kubické



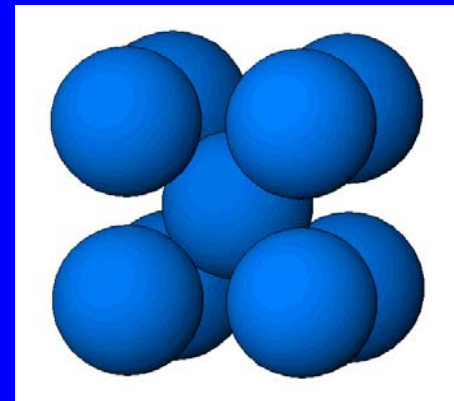
Mg, Be, Zn, Ni, Li, Be, Os, He



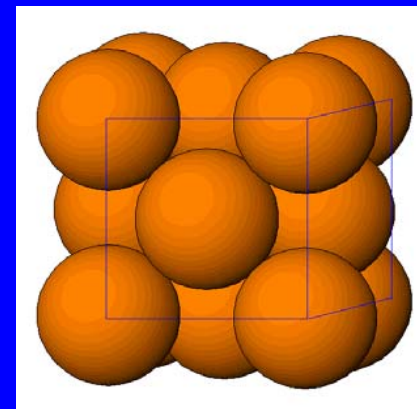
(a)



(b)



hexagonální

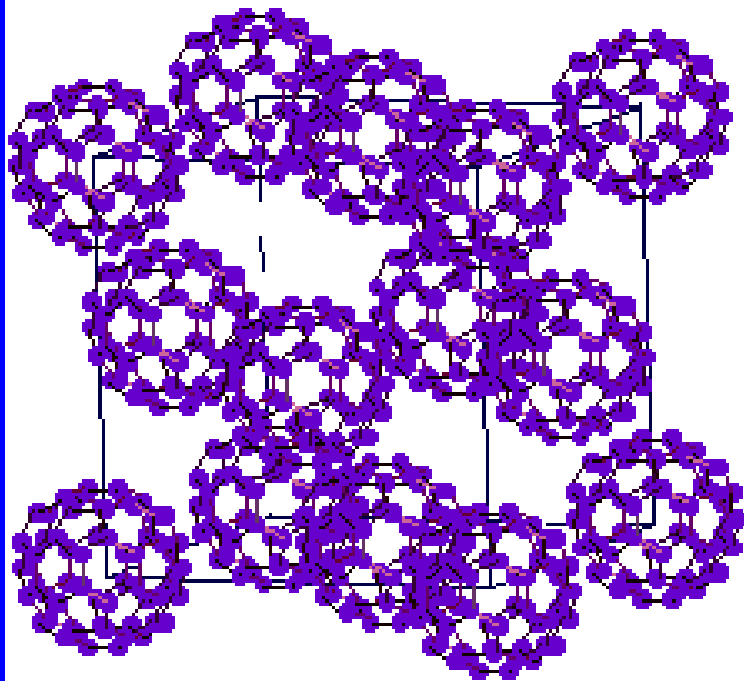


kubické

**Cu, Ca, Sr, Ag, Au, Ar, F₂, C₆₀,
opal (300 nm)**

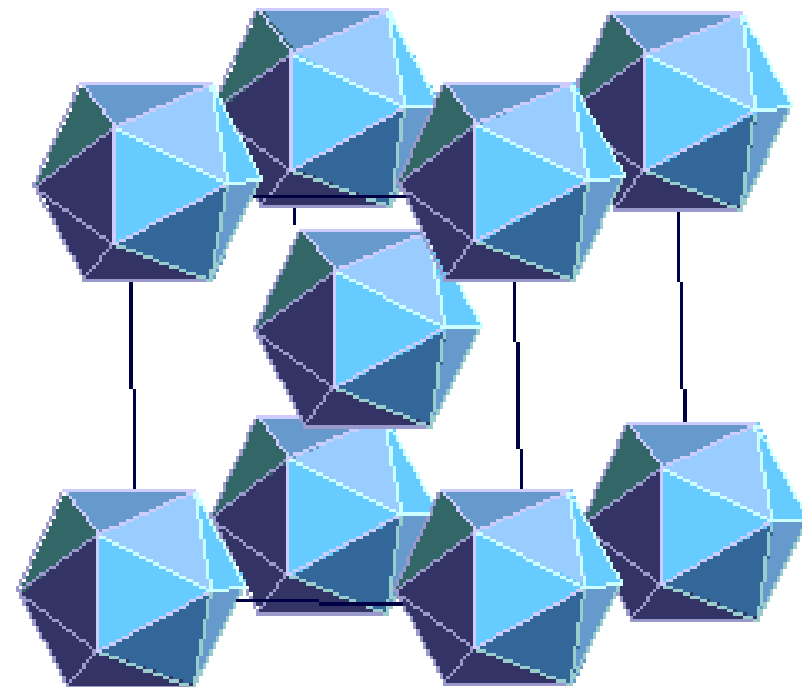
Struktury z velkých částic

BUCKMINSTERFULLERENE

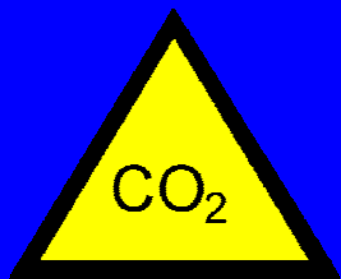


FCC

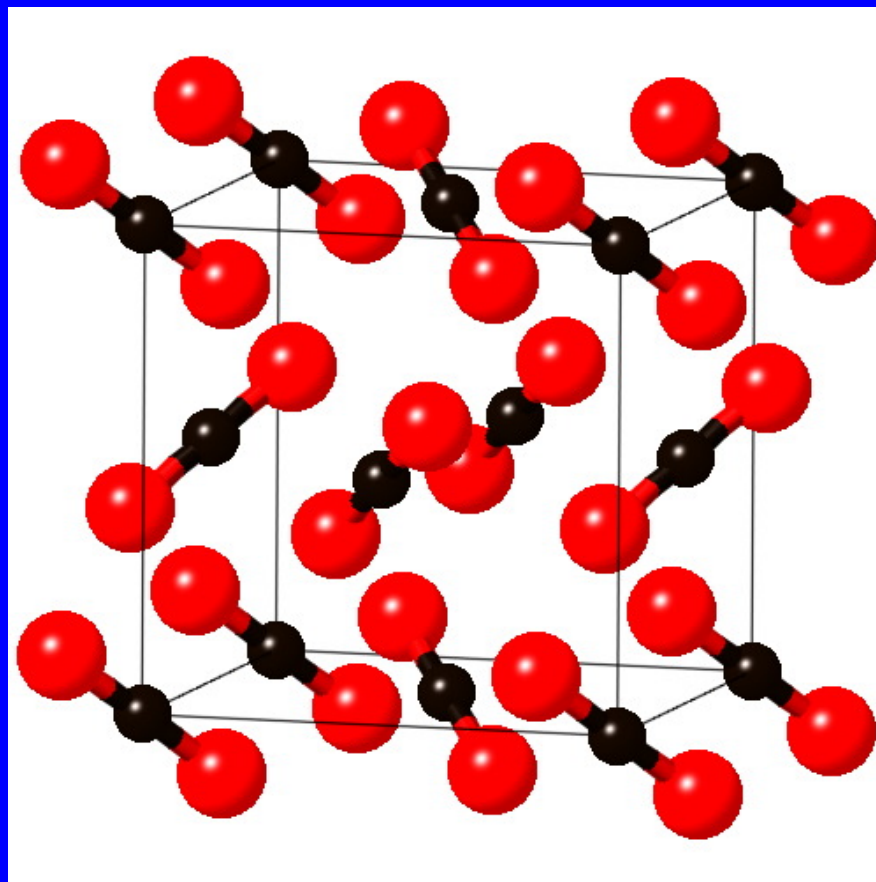
FOOT & MOUTH VIRUS



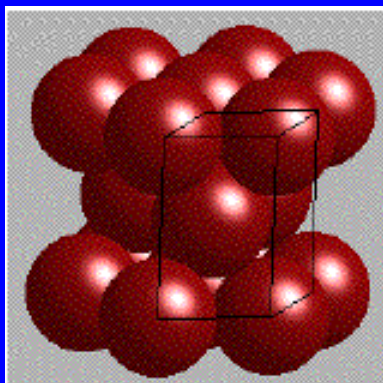
BCC



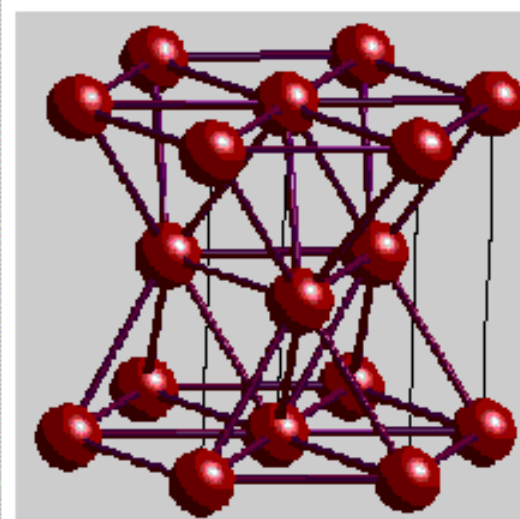
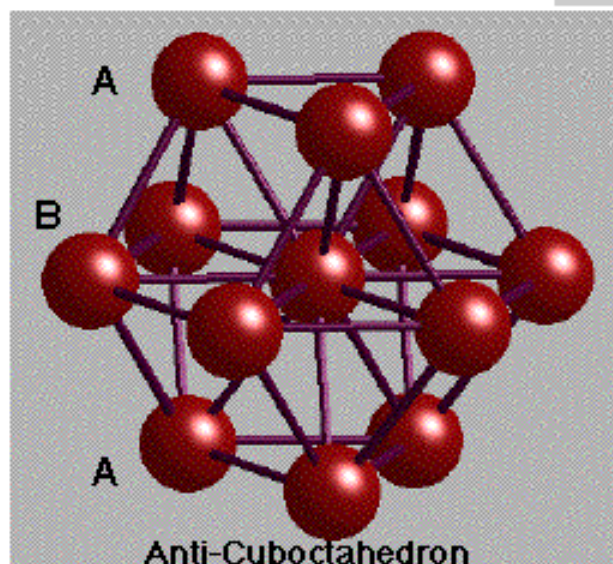
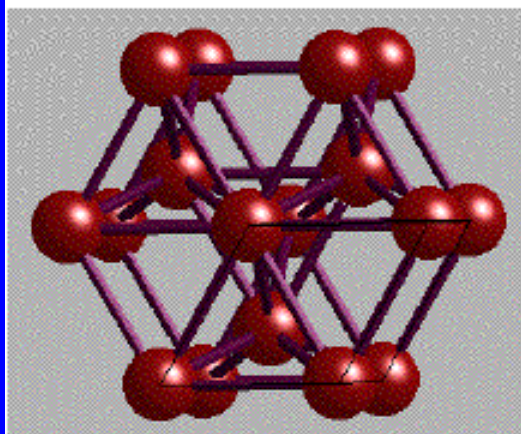
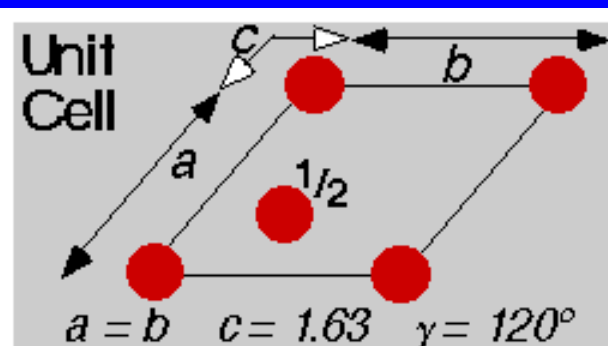
Struktura suchého ledu



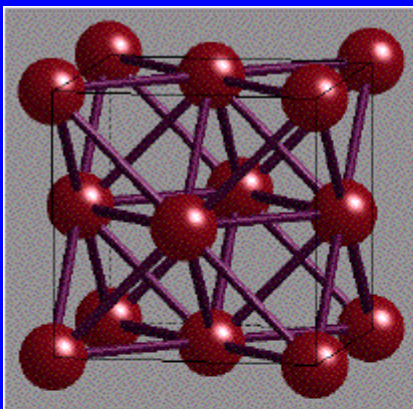
Nejtěsnější hexagonální uspořádání



HEXAGONAL CLOSE-PACKING

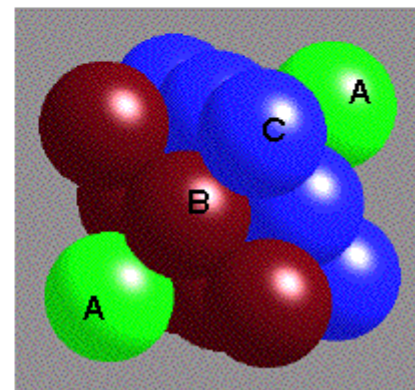
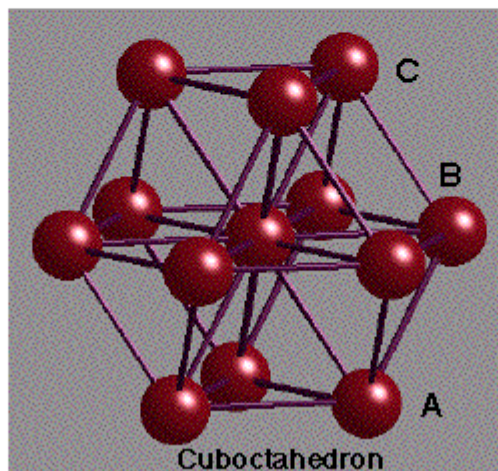
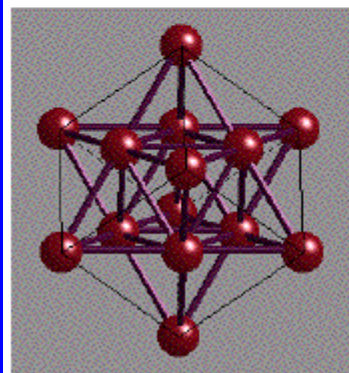
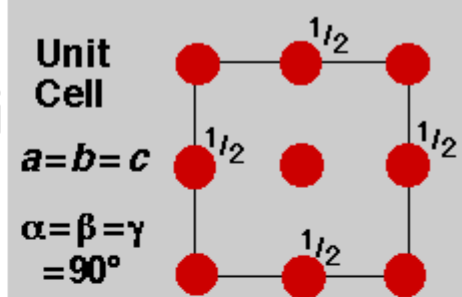


Nejtěsnější kubické uspořádání

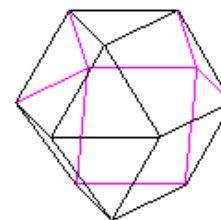
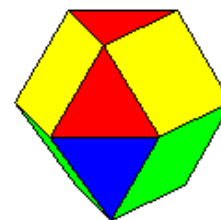
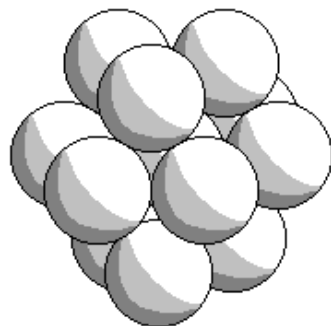
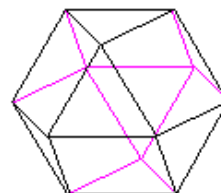
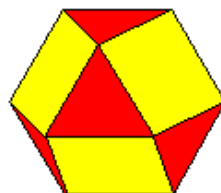
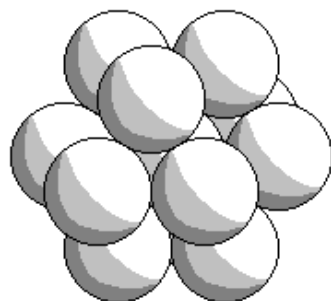
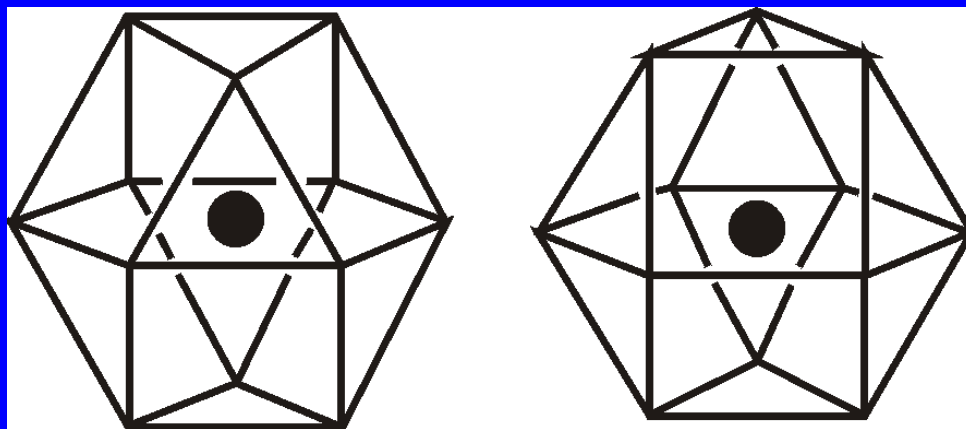


CUBIC CLOSE-PACKING

Face-Centred Cubic
(FCC) Unit Cell



Koordinální polyedry



Primitivní buňka

$$Z = 1$$

Tělesně centrovaná buňka

$$Z = 2$$

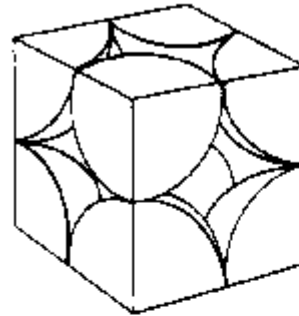
**Nejtěsnější hexagonální
uspořádání**

**Nejtěsnější kubické
uspořádání**

$$Z = 4$$

Typ uspořádání	Packing Efficiency	Coordination Number
----------------	--------------------	---------------------

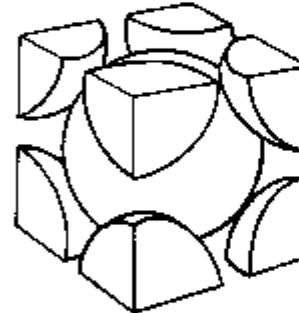
Simple cubic (sc)



52%

6

Body-centered cubic (bcc)



68%

8

Hexagonal close-packed (hcp)

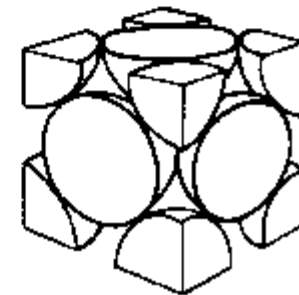
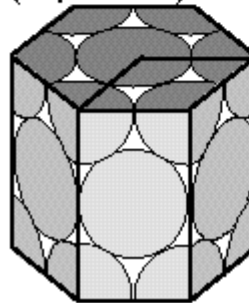
74%

12

Cubic close-packed (ccp or fcc)

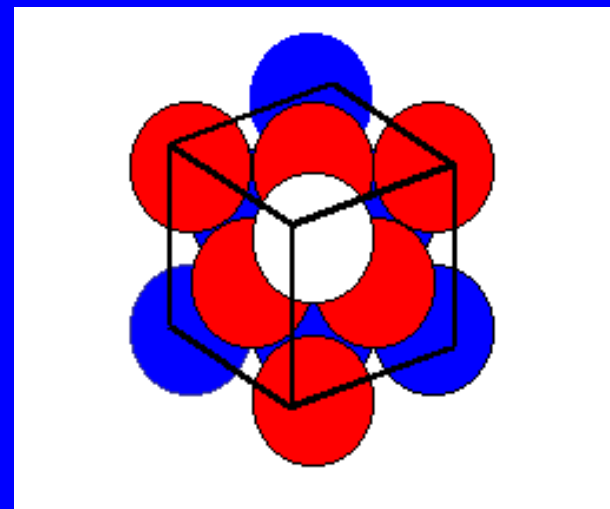
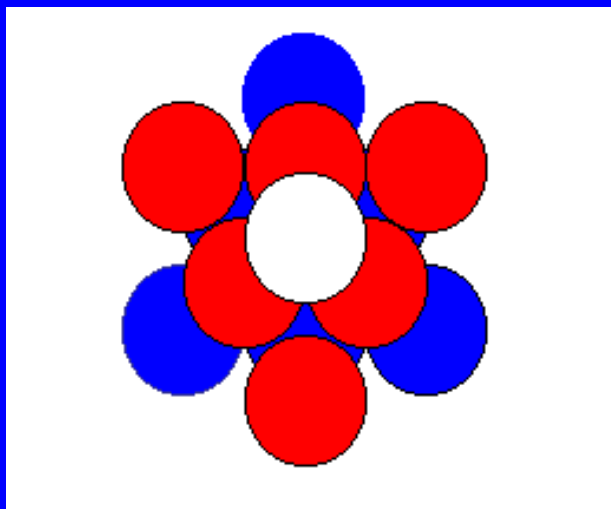
74%

12

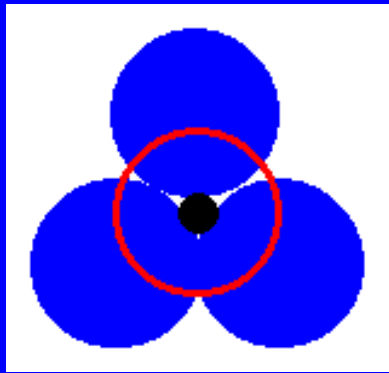


Nejtěsnější kubické uspořádání = plošně centrovaná buňka

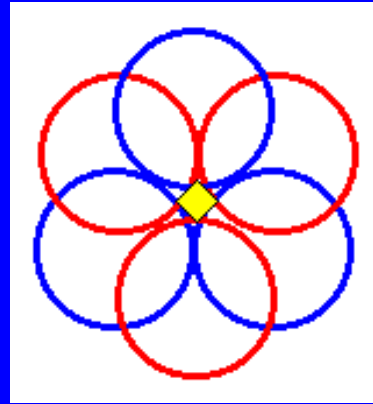
Skládání vrstev (ABC)



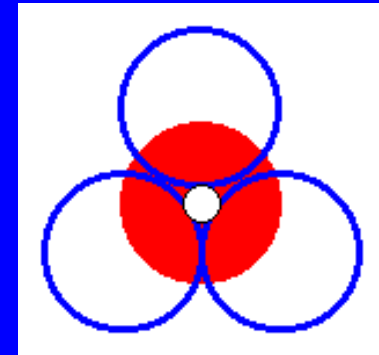
Nejtěsněji uspořádané vrstvy jsou orientovány kolmo k tělesové
diagonále kubické buňky



Tetraedrické T_+

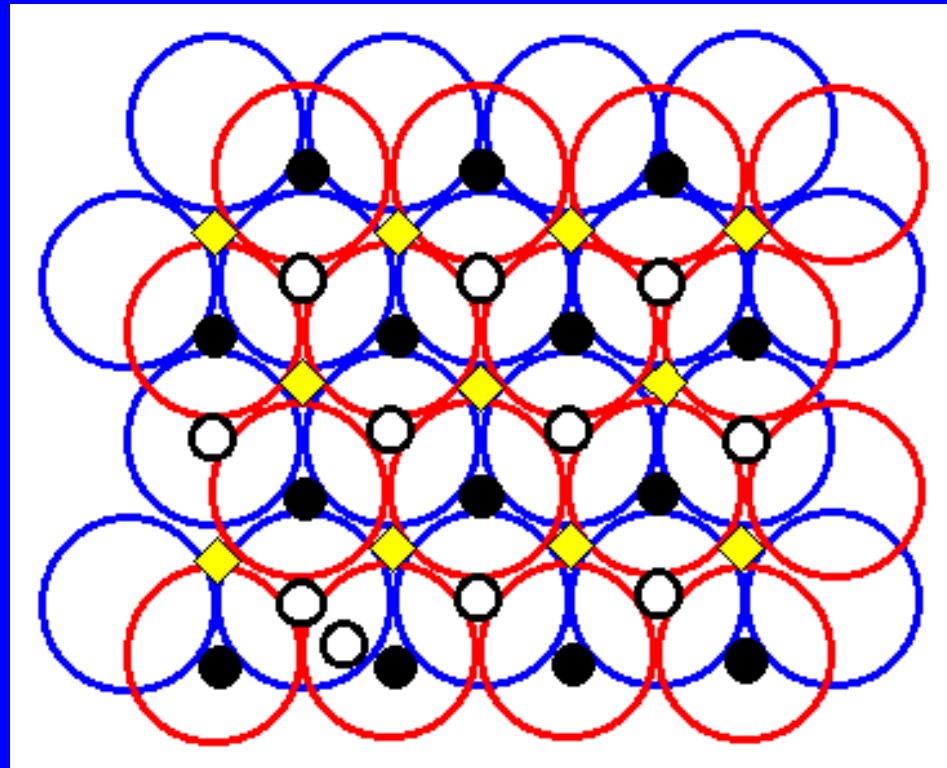


Oktaedrické O



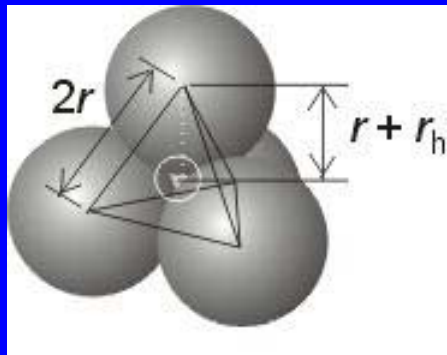
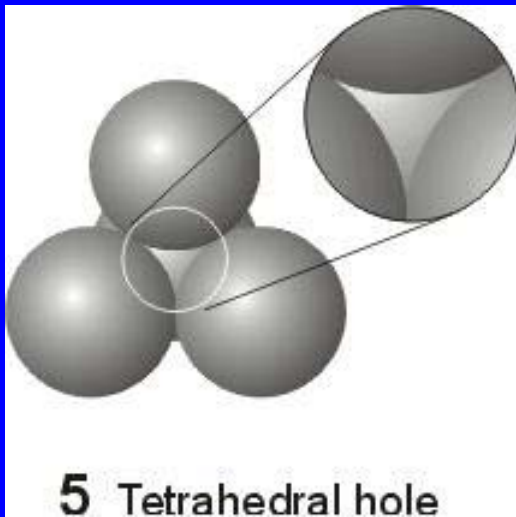
Tetraedrické T_-

Na N nejtěsněji
 uspořádaných atomů v
 buňce připadá N
 oktaedrických a $2N$
 tetraedrických mezer

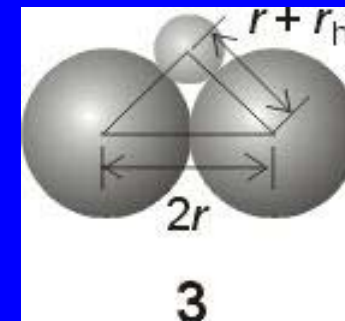
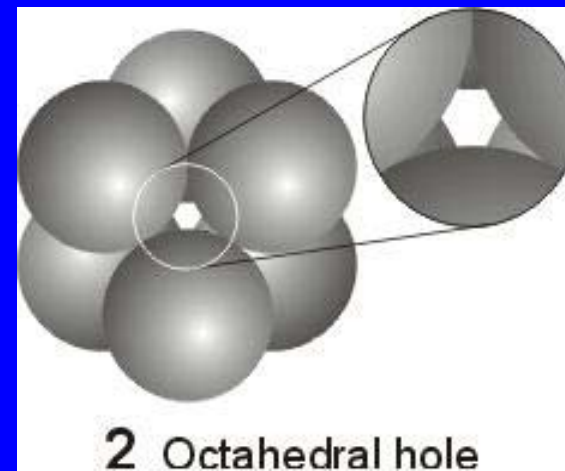


Dva typy mezer

Tetraedrické mezery ($2N$)



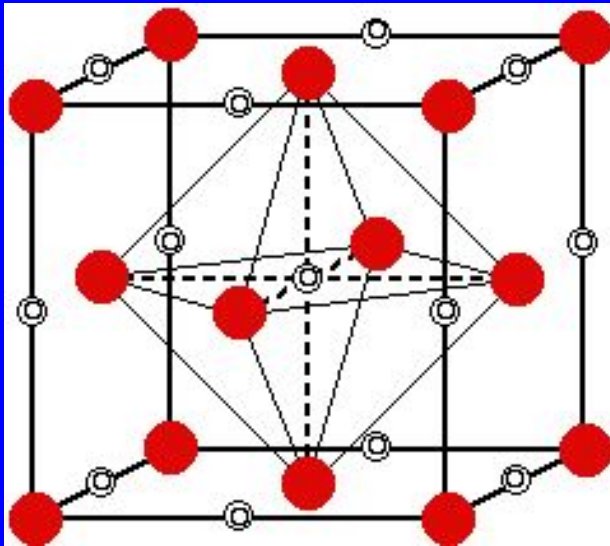
Oktaedrické mezery (N)



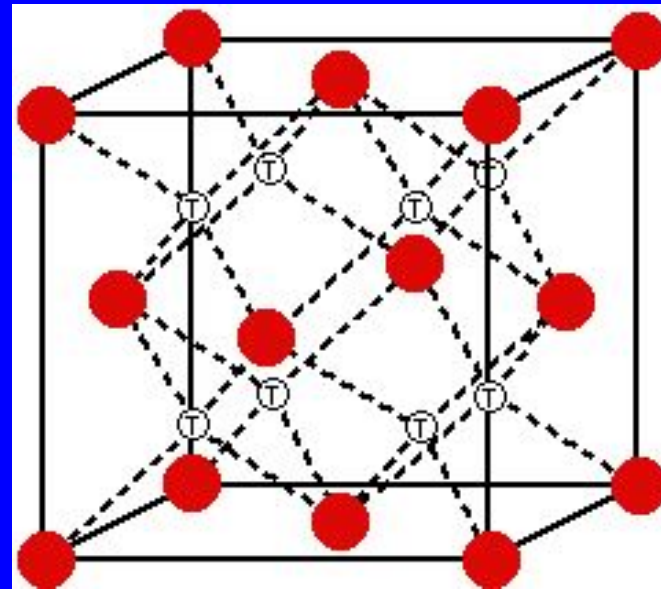
Dva typy mezer

Nejtěsnější kubické uspořádání = plošně centrovaná buňka

Počet atomů v buňce $N = 4$

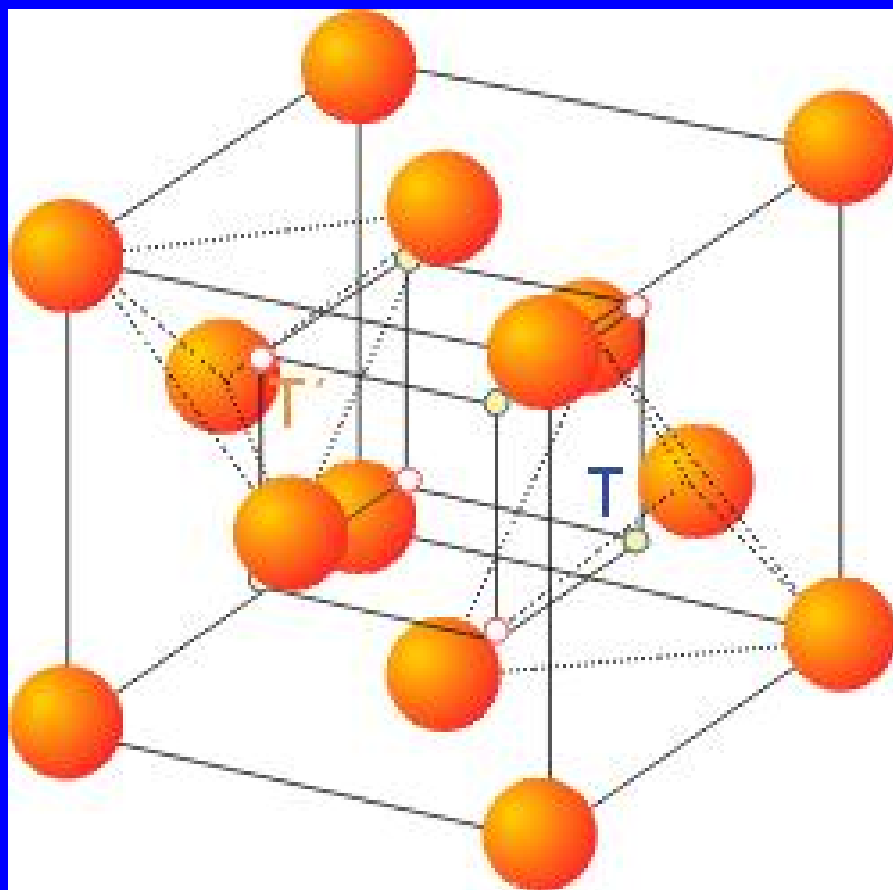


Oktaedrické mezery ($N = 4$)



Tetraedrické mezery ($2N = 8$)

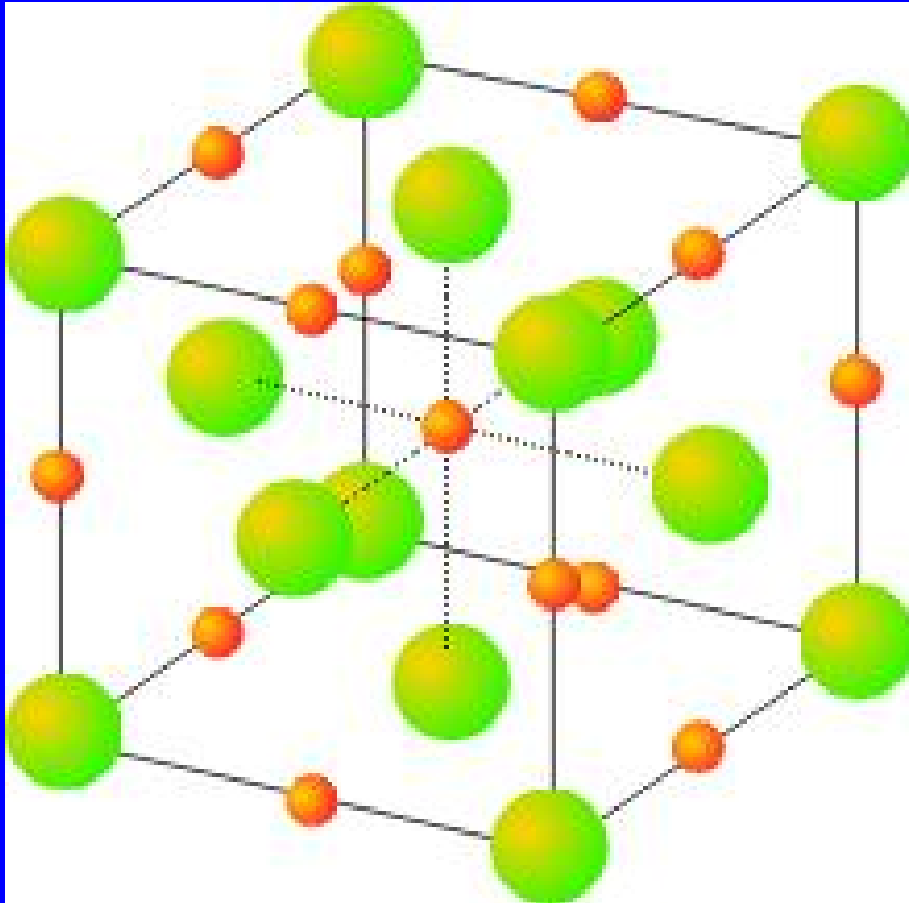
Tetraedrické mezery (2N)



$Z = 4$
počet atomů v buňce

$N = 8$
počet tetraedrických
mezer

Oktaedrické mezery (N)

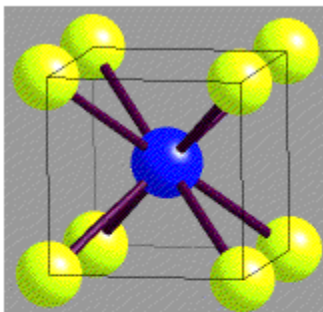


$Z = 4$
počet atomů v buňce

$N = 4$
počet oktaedrických
mezer

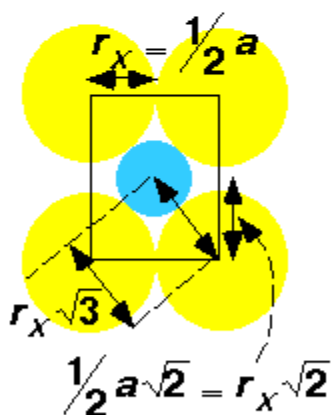
Limiting Radius Ratios

CsCl 8:8



unit cell

cell side a

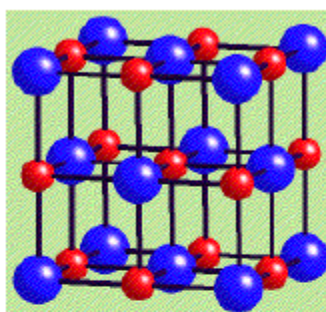


$$r_M + r_X = r_X \sqrt{3}$$

$$r_M / r_X = \sqrt{3} - 1$$

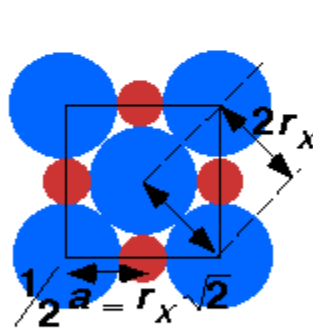
$$= 0.732$$

NaCl 6:6



unit cell

face diagonal $a\sqrt{2}$

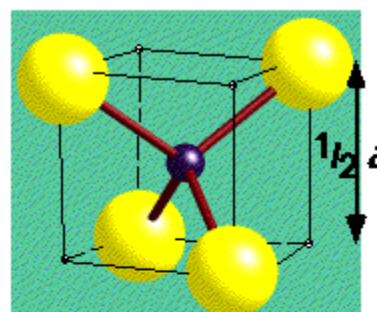


$$r_M + r_X = r_X \sqrt{2}$$

$$r_M / r_X = \sqrt{2} - 1$$

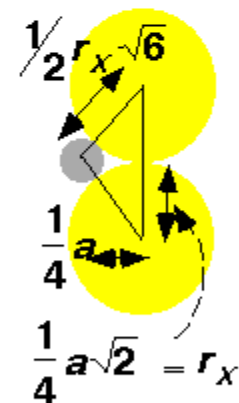
$$= 0.414$$

ZnS 4:4



1/8th unit cell

body diagonal $a\sqrt{3}$

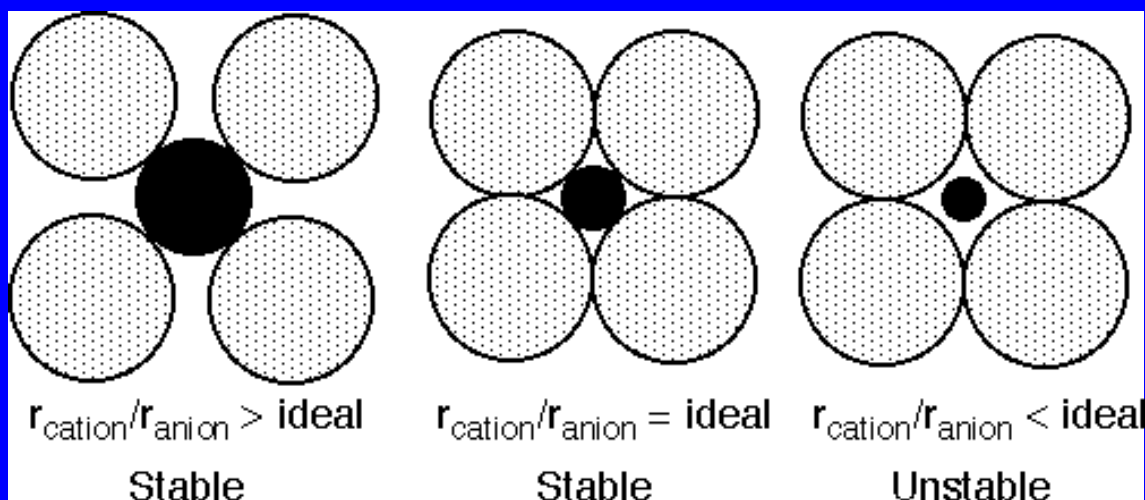


$$r_M + r_X = \frac{1}{2} r_X \sqrt{6}$$

$$r_M / r_X = \frac{1}{2} \sqrt{6} - 1$$

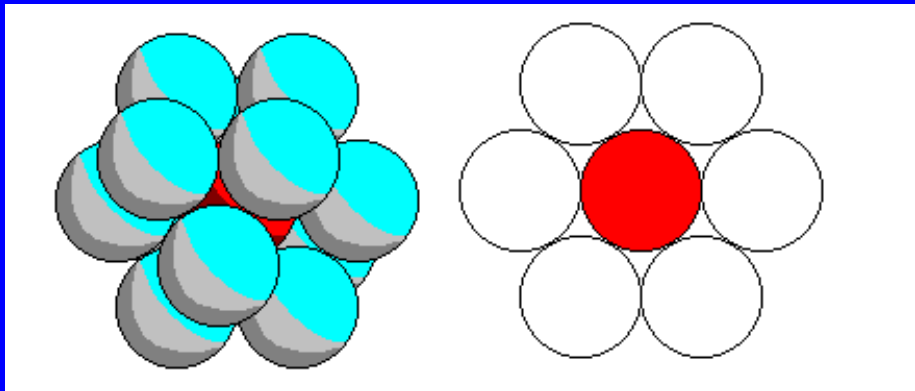
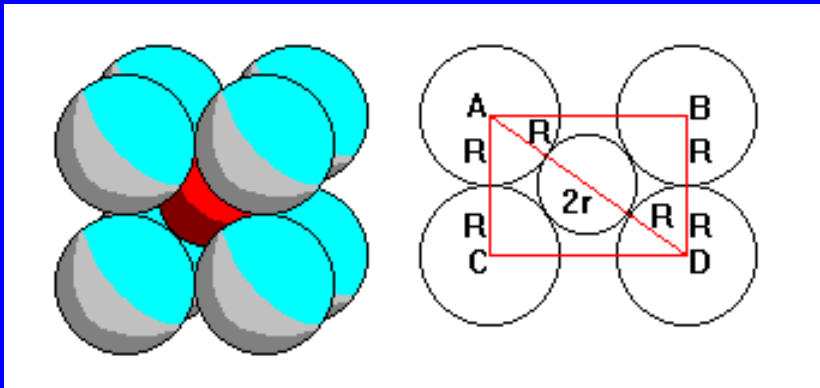
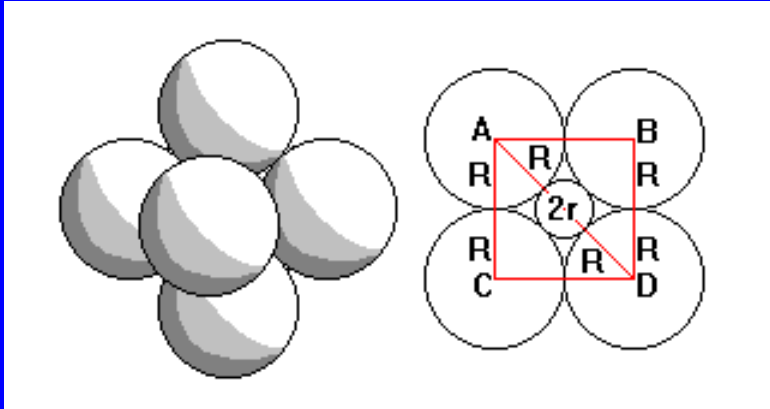
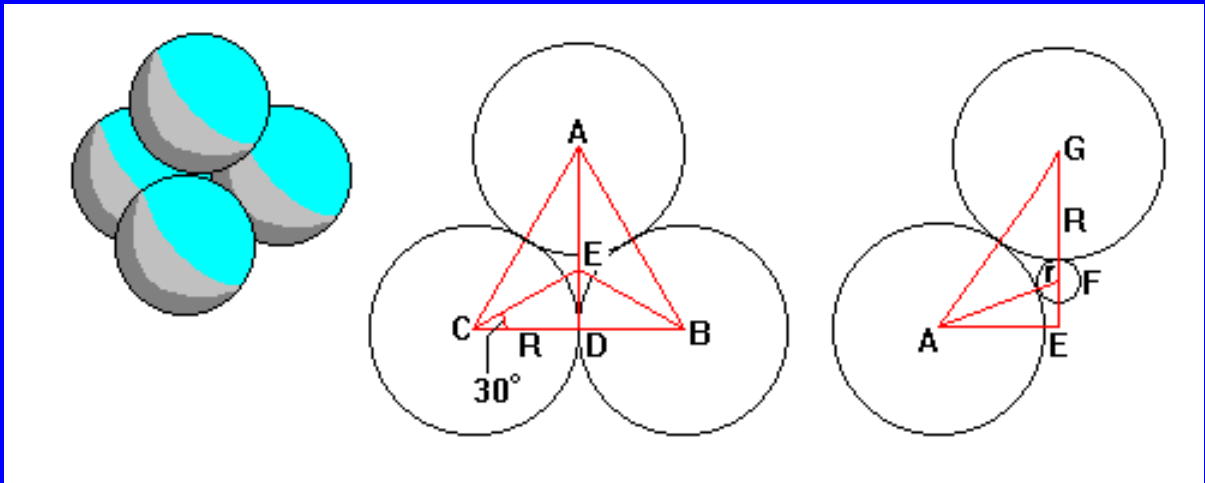
$$= 0.225$$

Poměr velikostí kationtu/aniontu

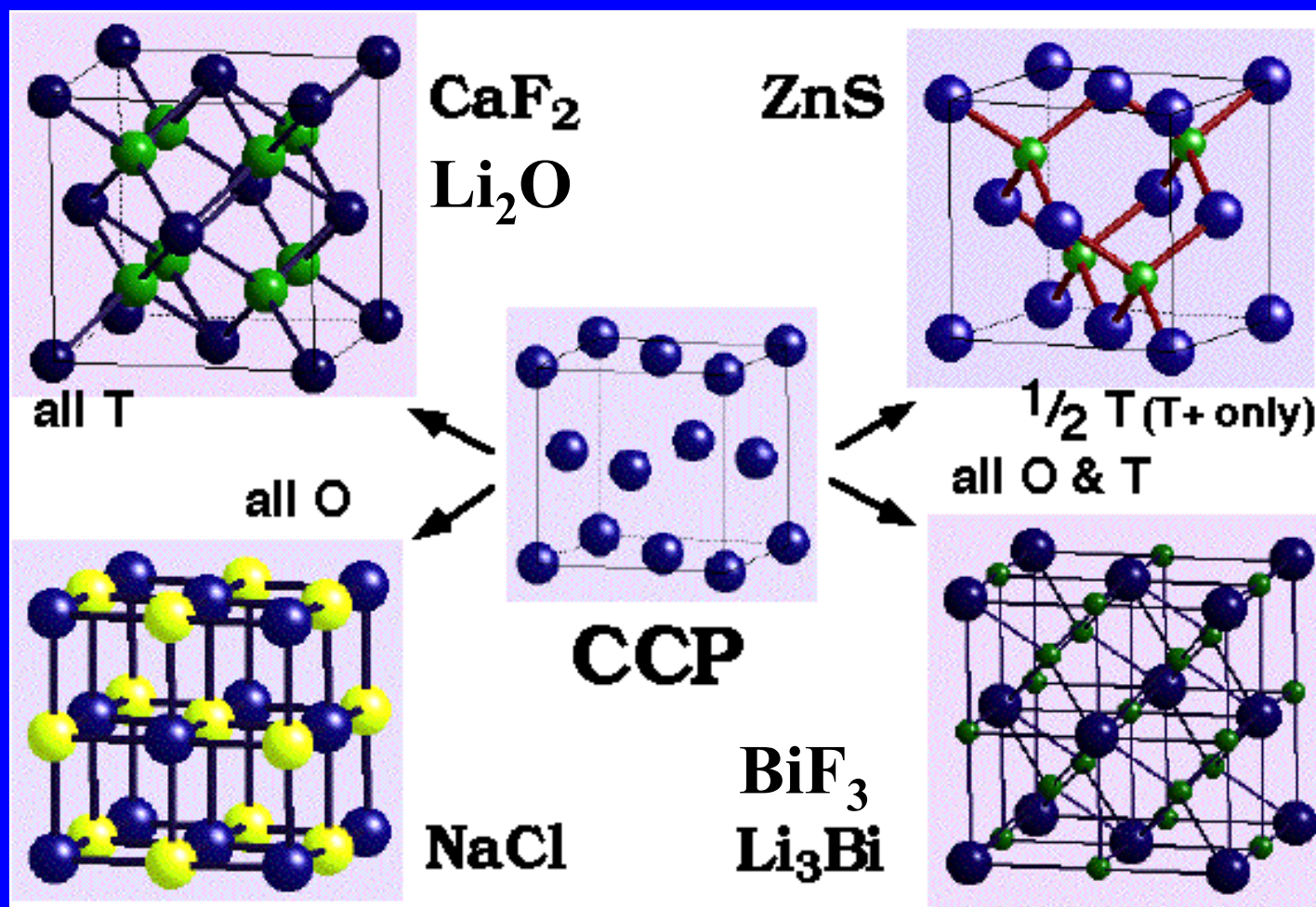


Koordinační č.	r/R
12 – kub. a hex.	1.00 (substituce)
8 – Kubická	0.732 – 1.00
6 – Oktaedrická	0.414 – 0.732
4 – Tetraedrická	0.225 – 0.414

↓
 Velikost
 mezery
 klesá



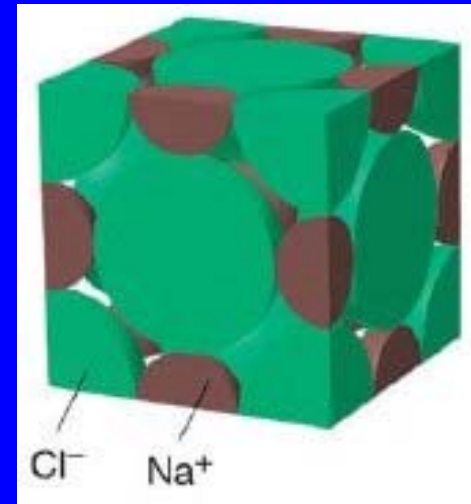
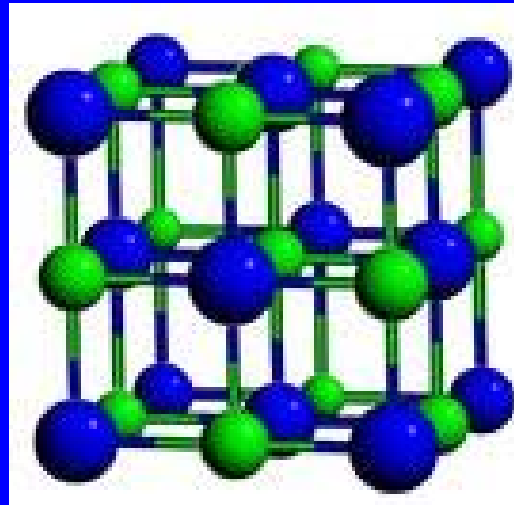
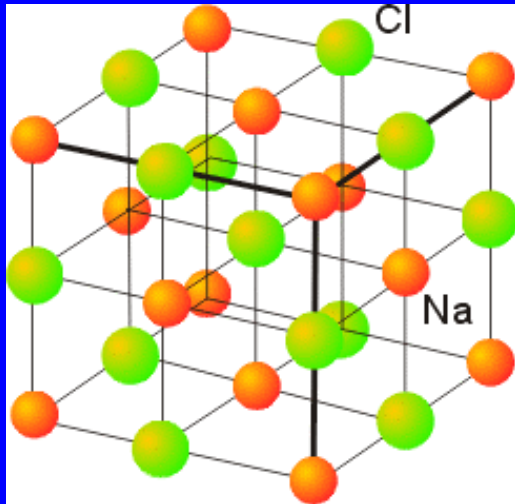
Struktury odvozené od nejtěsnějšího kubického uspořádání



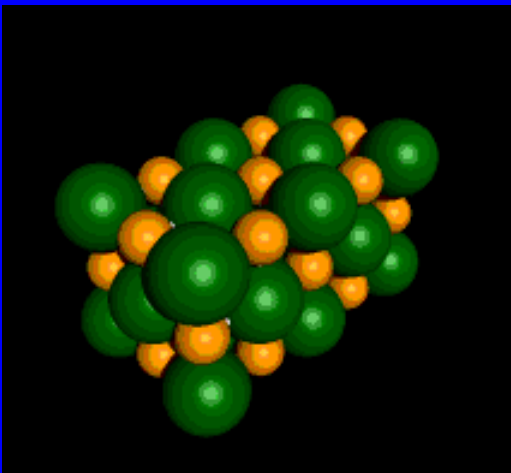
Struktury odvozené od nejtěsnějšího kubického uspořádání

Anionty/buňku (= 4)	Okt. (Max 4)	Tet. (Max 8)	Stechiometrie	Příklady
4	100% = 4	0	$M_4X_4 = MX$	NaCl (6:6 koord.)
4	0	100% = 8	$M_8X_4 = M_2X$	Li ₂ O (4:8 koord.)
4	0	50% = 4	$M_4X_4 = MX$	ZnS, sfalerit (4:4 koord.)
4	50% = 2	0	$M_2X_4 = MX_2$	CdCl ₂
4	100% = 4	100% = 8	$M_{12}X_4 = M_3X$	Li ₃ Bi
4	50% = 2	12.5% = 1	M_3X_4	MgAl ₂ O ₄ , spinel

Chlorid sodný, NaCl

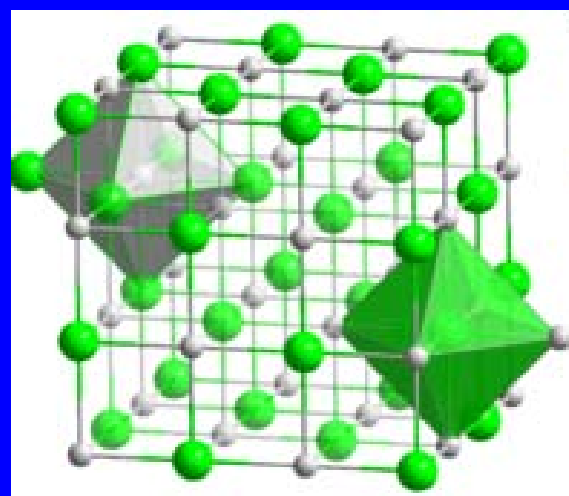
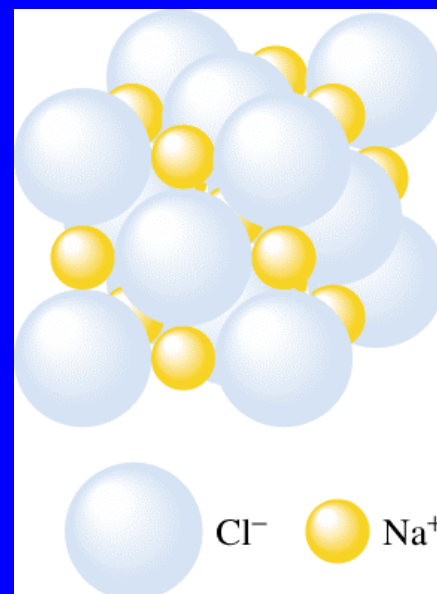
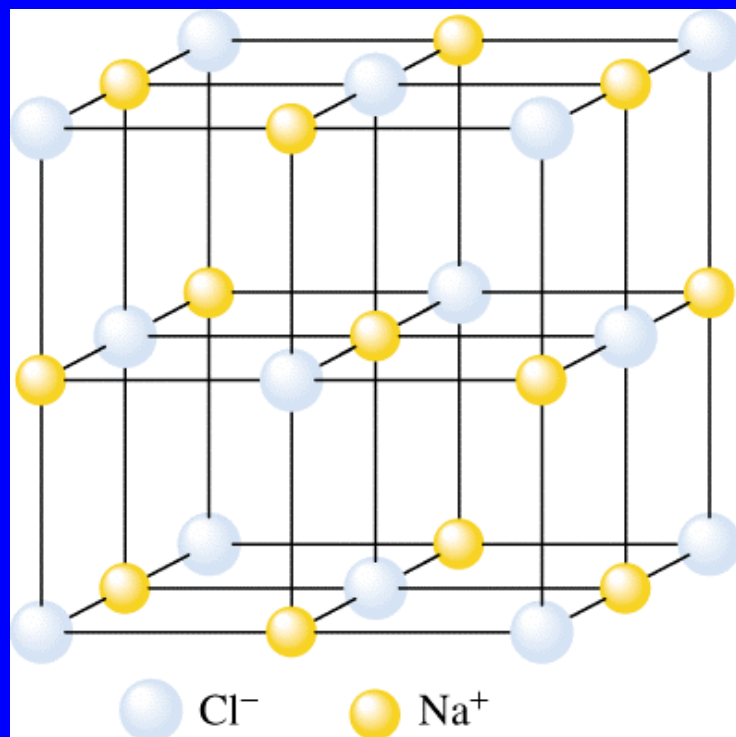


$Z = ?$

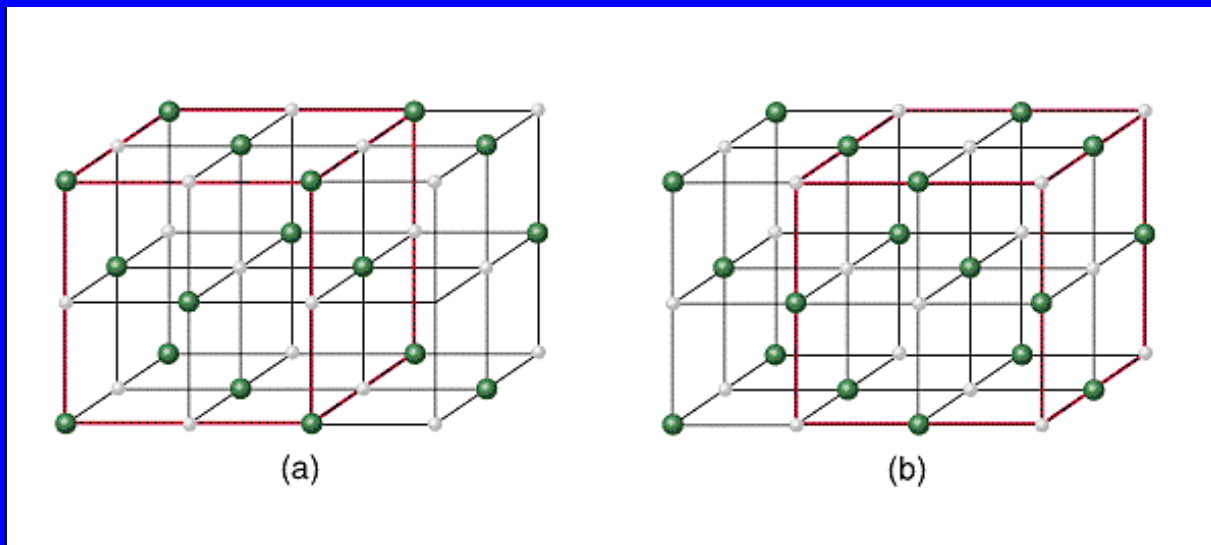
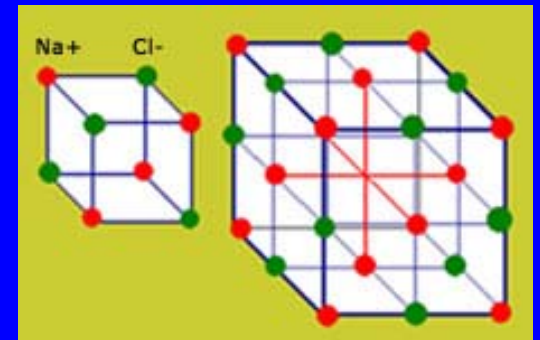
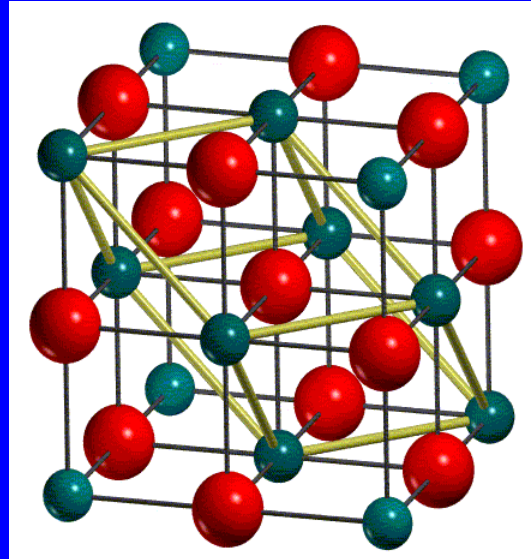
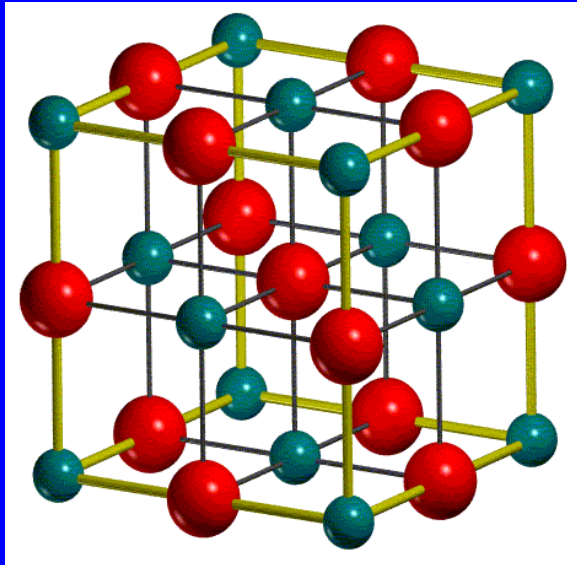


Nejtěsnější kubické uspořádání Cl,
Na obsazuje oktaedrické mezery

Chlorid sodný, NaCl



Koordinační číslo:
Na = 6
Cl = 6



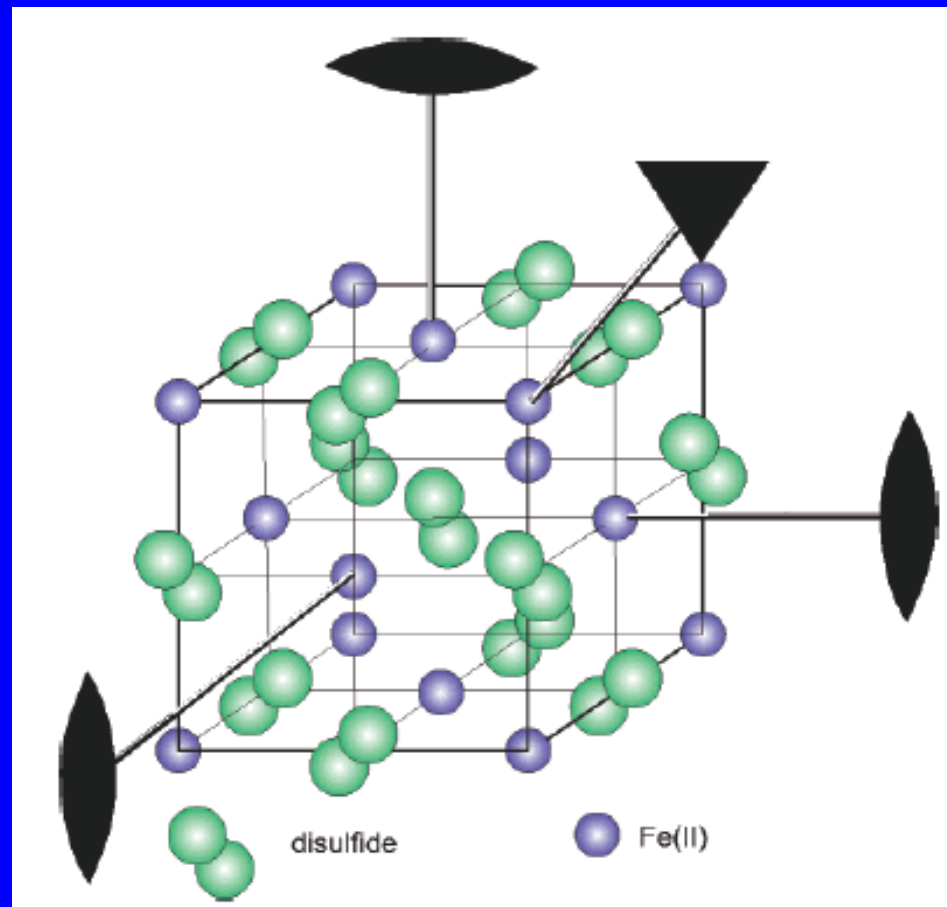
Dvě stejné nejtěsněji uspořádané kubické mřížky kationtů a aniontů

Struktura pyritu - FeS_2

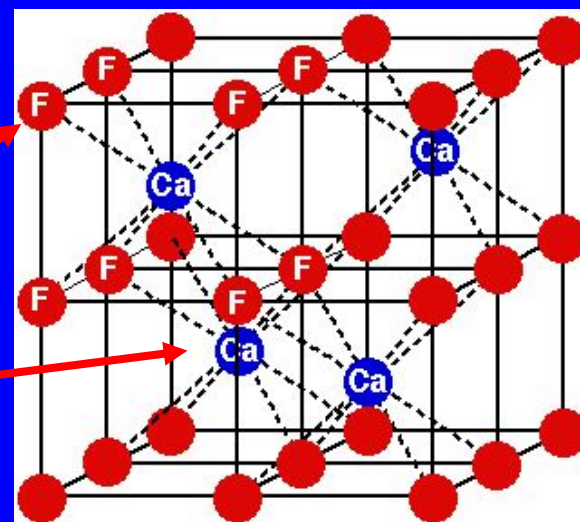
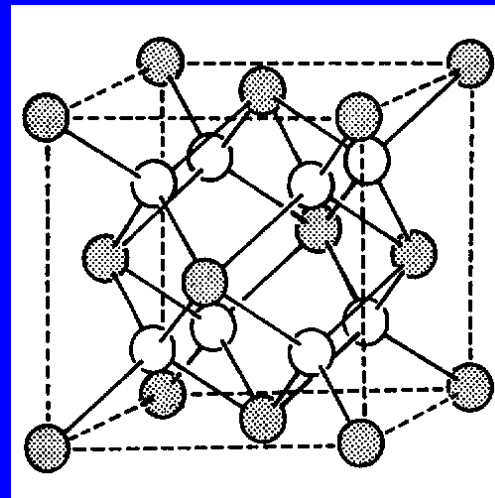
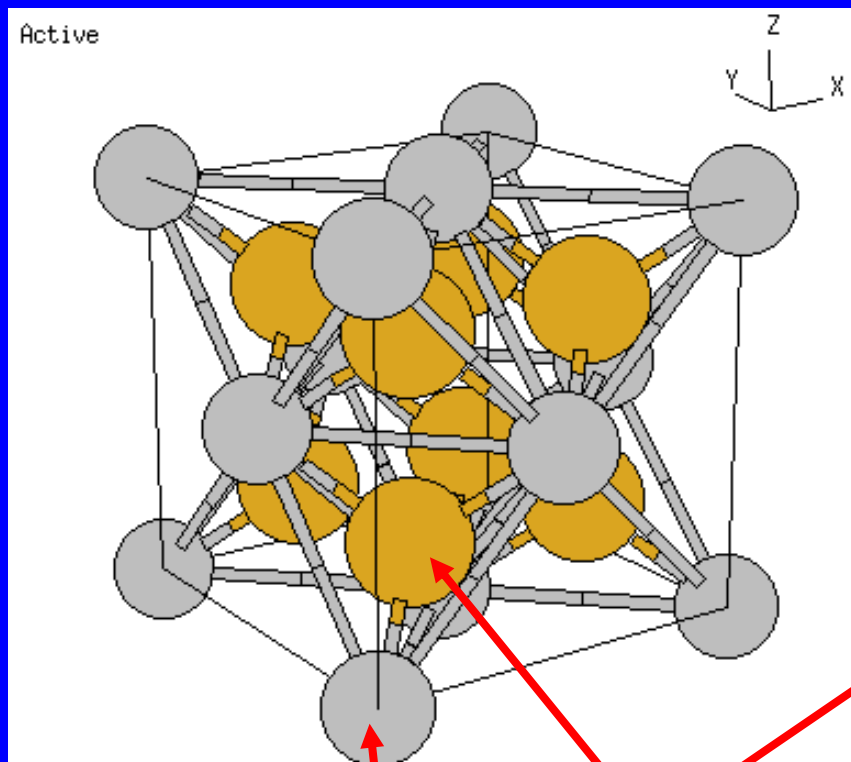
Odvození složitějších struktur od jednoduchých strukturních typů

Na^+ Cl^-

Fe^{2+} S_2^{2-}



Fluorit, CaF_2 (inverzní typ Li_2O)



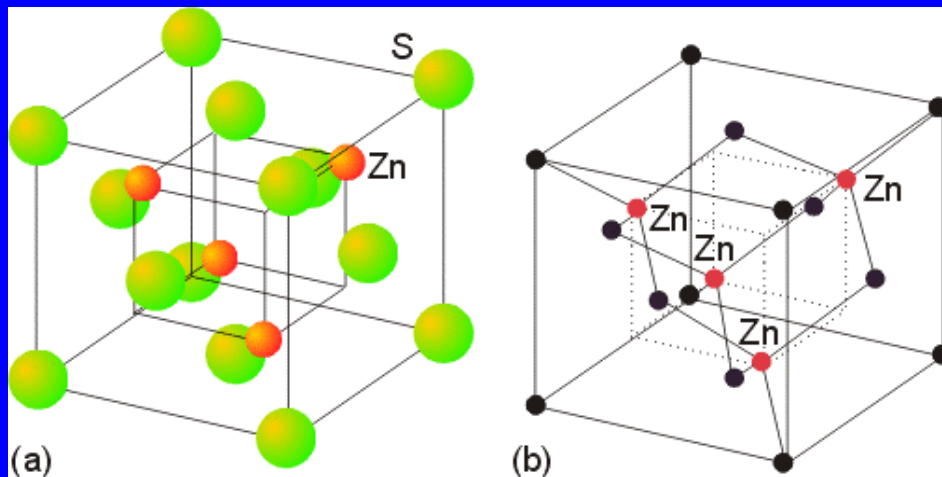
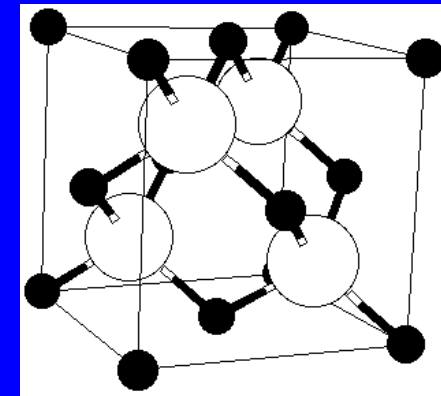
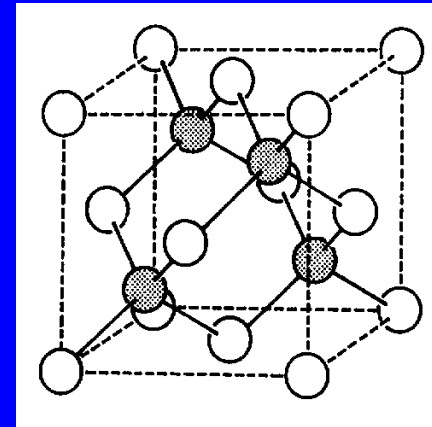
Ca / O
F / Li

$\text{K}_2[\text{PtCl}_6]$, $\text{Cs}_2[\text{SiF}_6]$, $[\text{Fe}(\text{NH}_3)_6][\text{TaF}_6]_2$

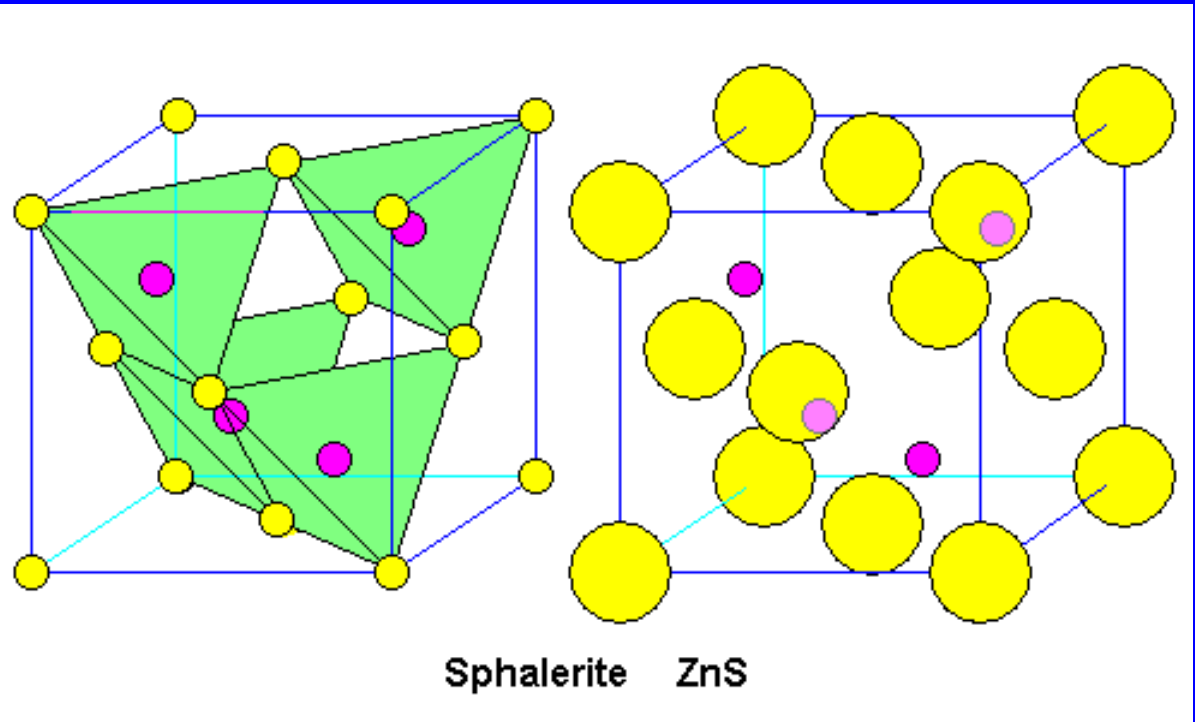
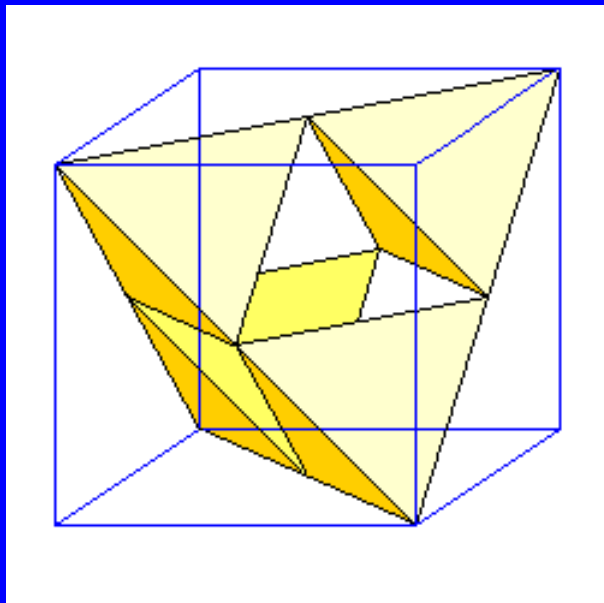
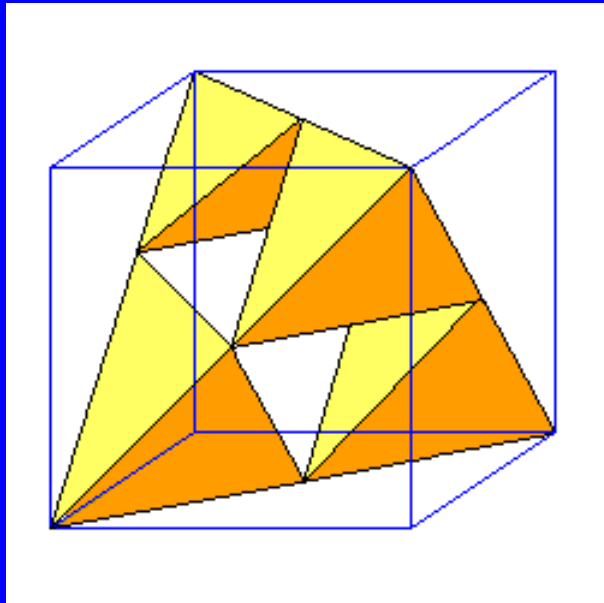
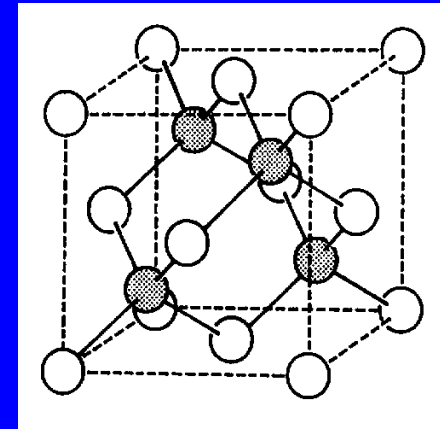
Sfalerit, ZnS

Nejtěsnější kubické uspořádání S
Zn obsazuje $\frac{1}{2}$ tetraedrických mezer

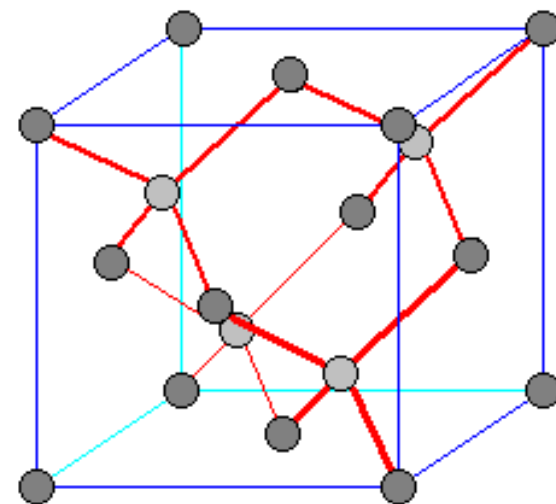
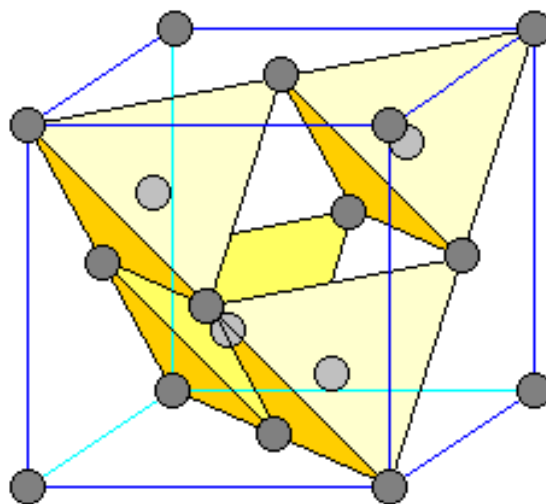
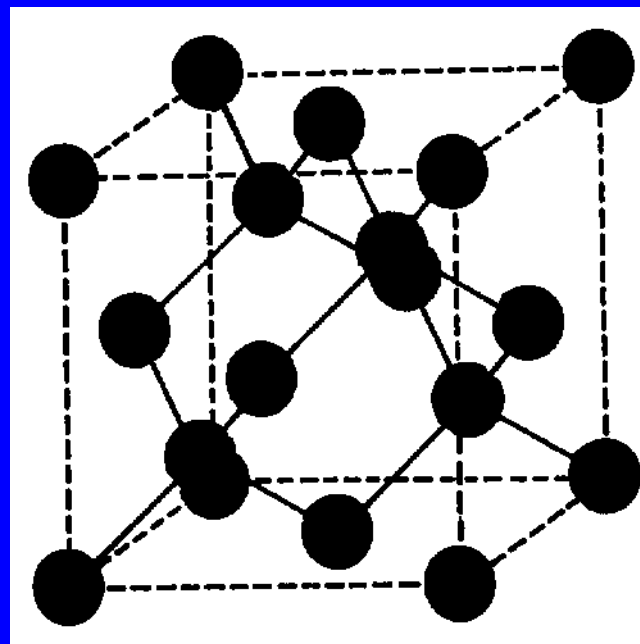
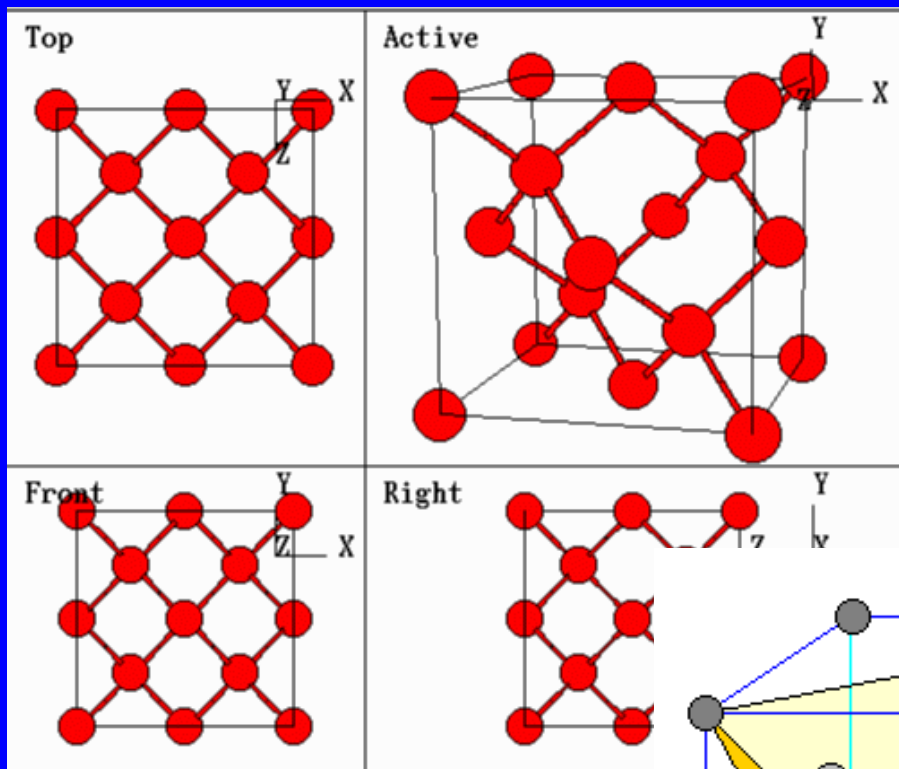
Nejtěsnější kubické uspořádání Zn
S obsazuje $\frac{1}{2}$ tetraedrických mezer



Sfalerit, ZnS



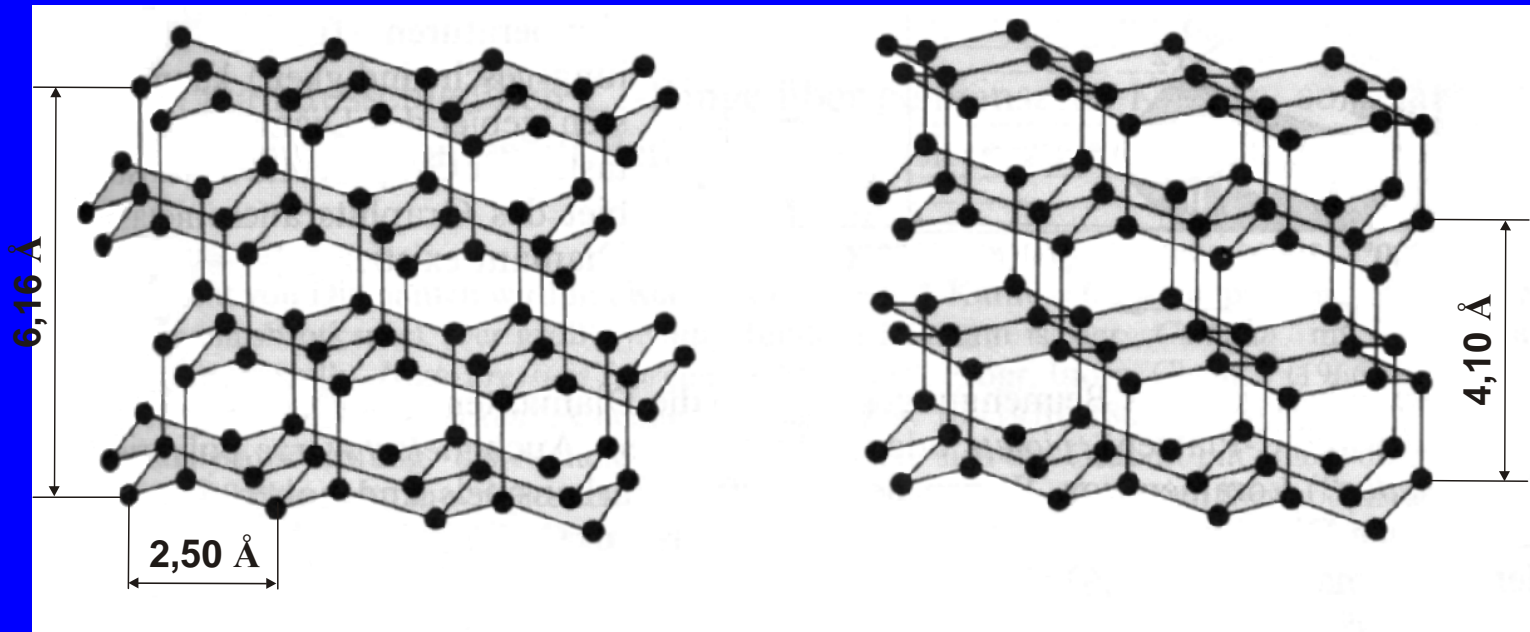
Diamant, C



Diamant, C

kubický

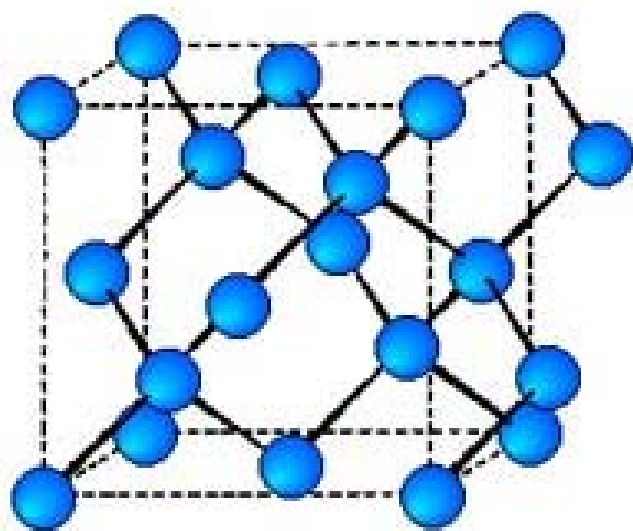
hexagonální
lonsdaleite



SiO₂ kristobalit

SiO₂ tridymit
led

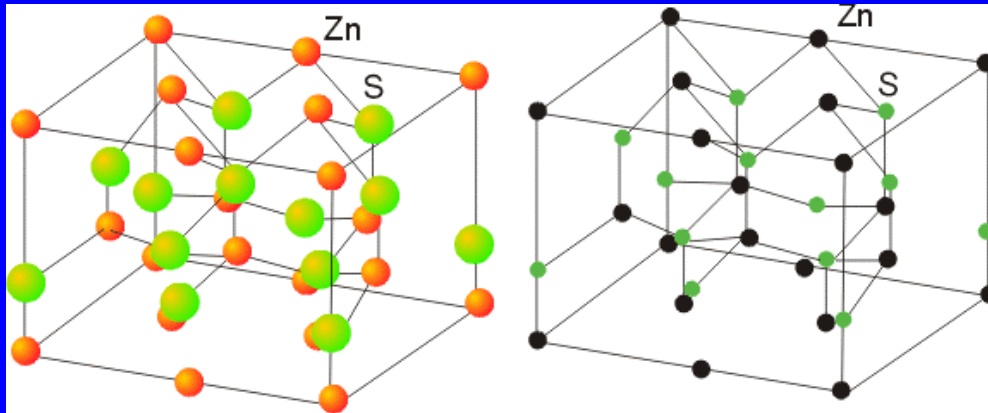
Struktura prvků 14. skupiny



	a (Å)	d (g.cm ⁻³)
C	3.566	3.515
Si	5.431	2.329
Ge	5.657	5.323
α -Sn	6.489	7.285

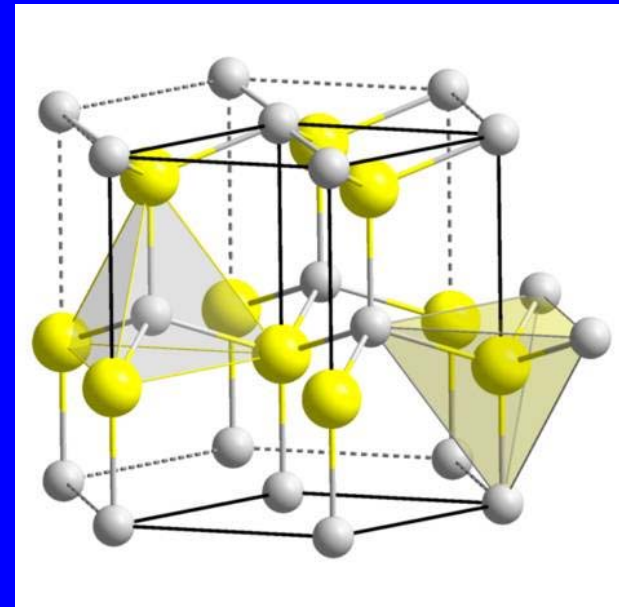
Stejná struktura – velikost buňky roste směrem dolů ve skupině

Wurzit, ZnS

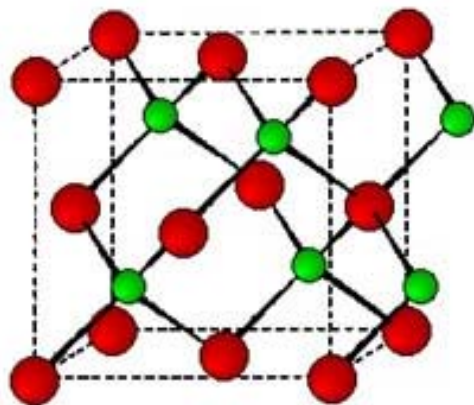


Nejtěsnější hexagonální
uspořádání S
Zn obsazuje
 $\frac{1}{2}$ tetraedrických mezer

Polymorfie ZnS



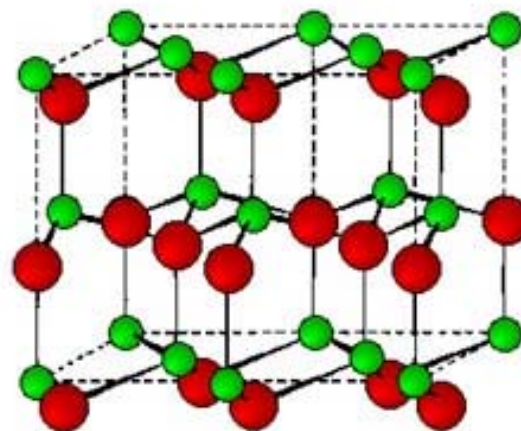
Polovodiče 13-15 a 12-16



Sfalerit

InP, GaAs

HgTe, CdTe

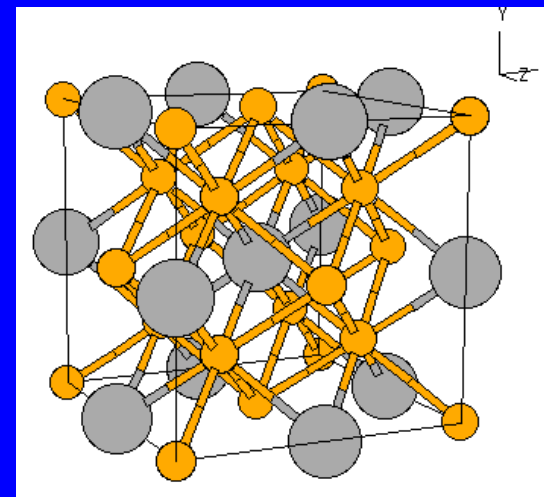
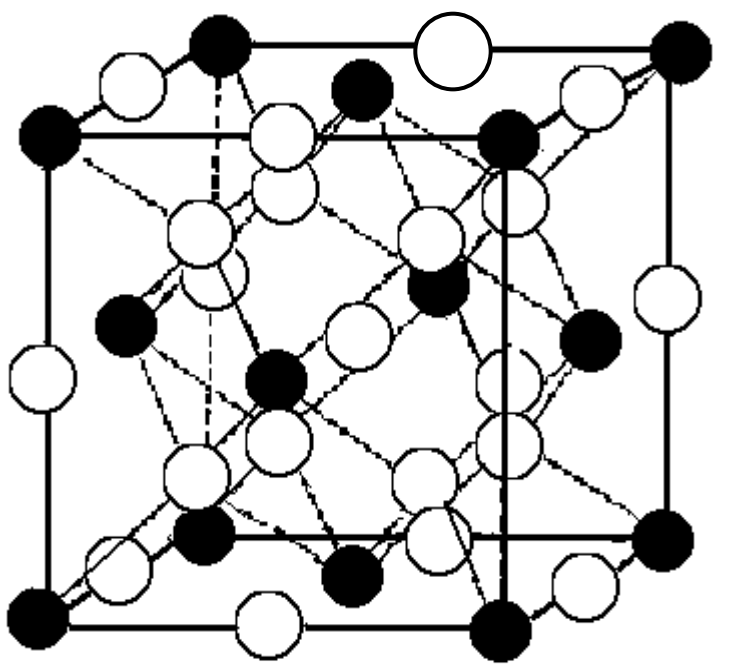


Wurzit

ZnO, CdSe

AlN, GaN

BiF₃/Li₃Bi

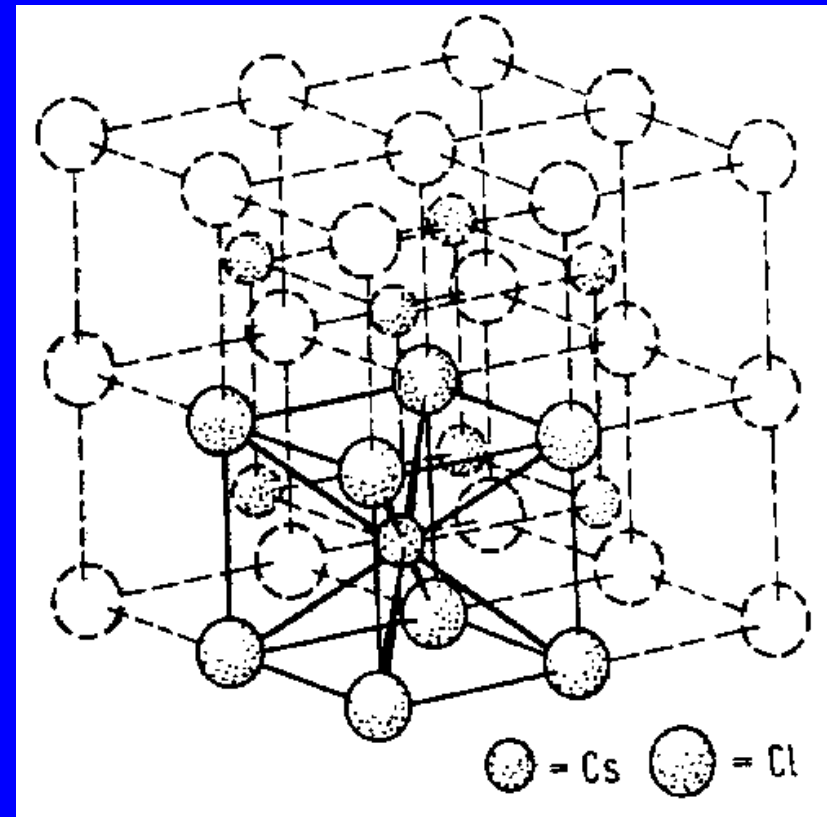
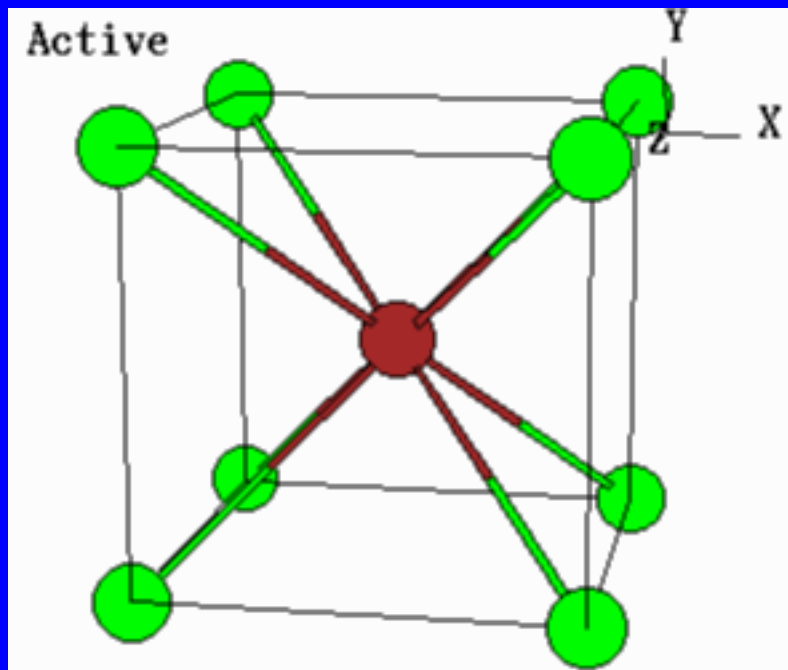
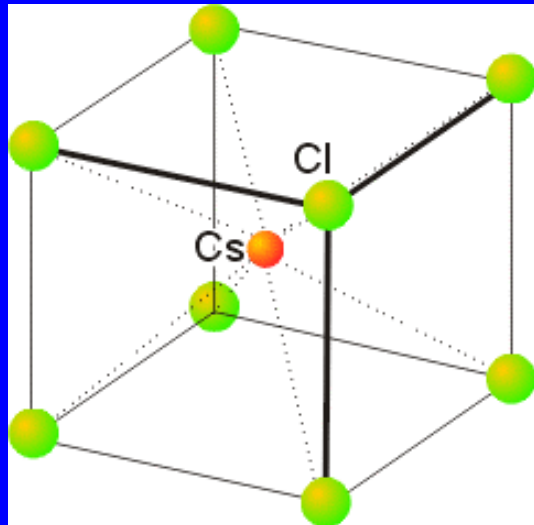


Nejtěsnější kubické uspořádání Bi (4)
F obsazuje tetraedrické mezery (8) a
oktaedrické mezery (4)

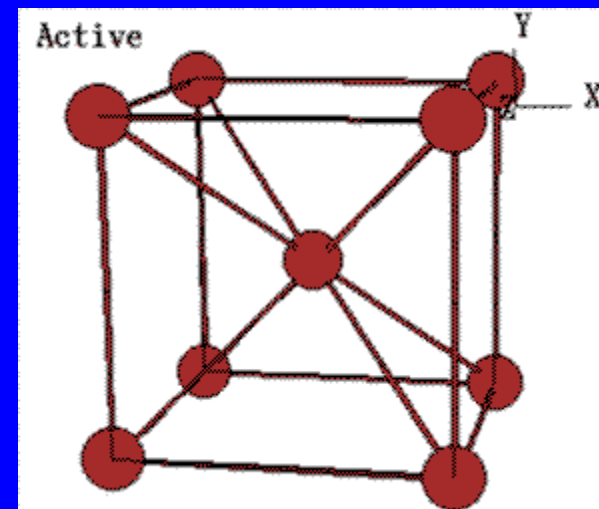
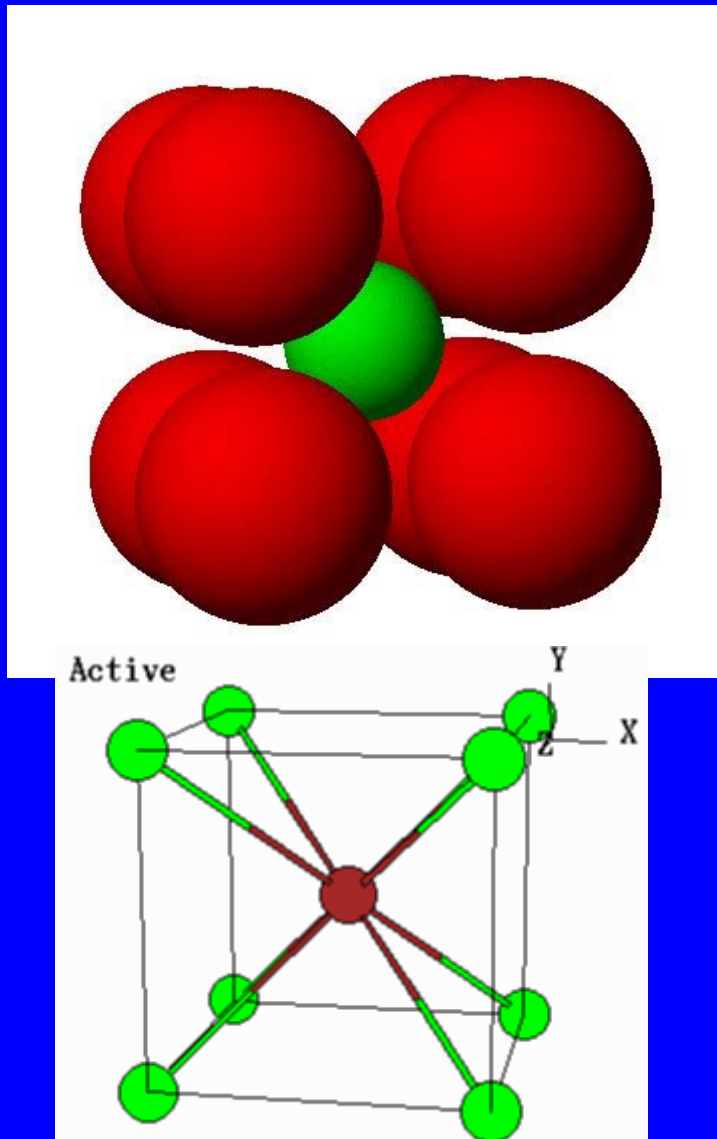
Nejtěsnější kubické uspořádání Bi (4)
Li obsazuje tetraedrické mezery (8) a
oktaedrické mezery (4)

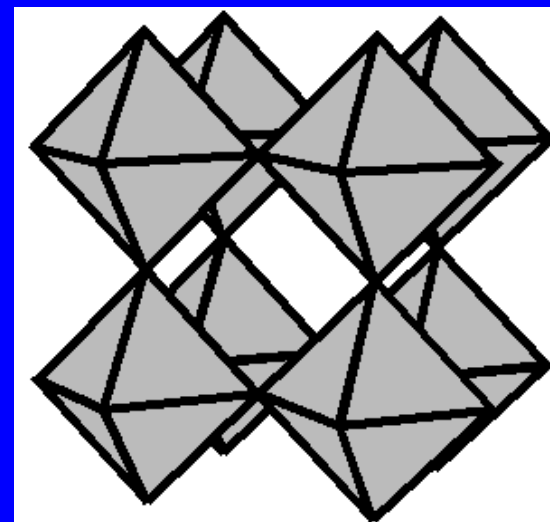
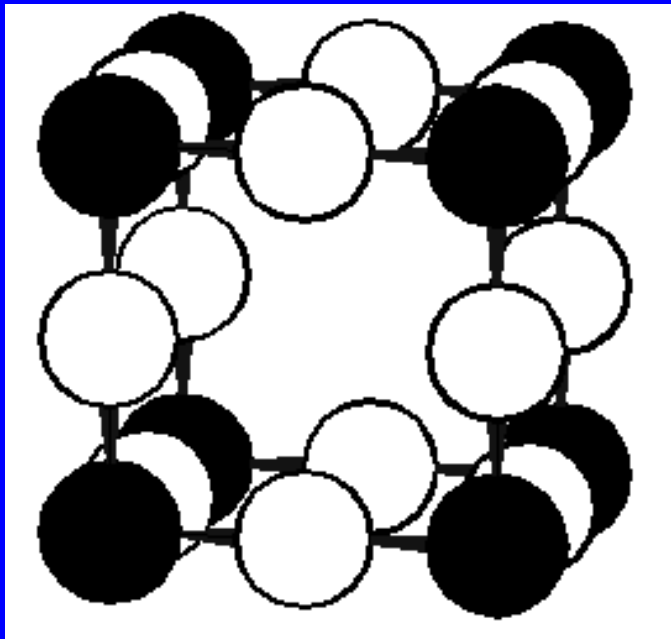


CsCl



CsCl není tělesně centrovaná
kubická buňka

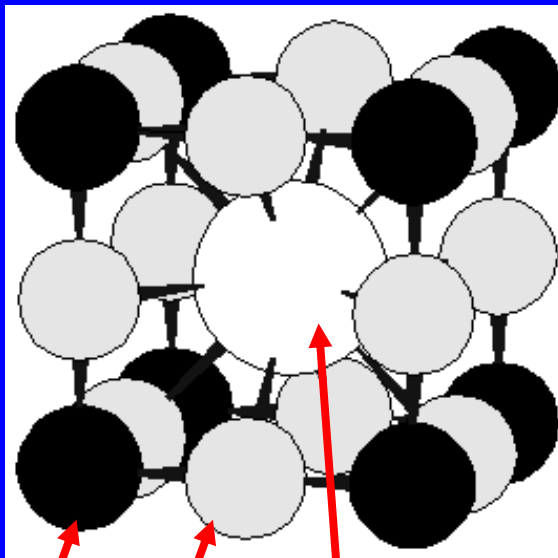




Primitivní kubická

Perovskit CaTiO_3

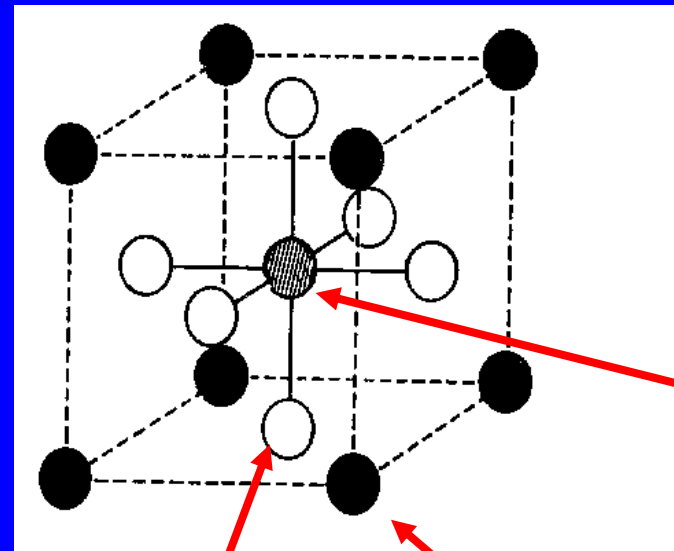
Dva ekvivalentní pohledy na základní buňku perovskitu



Ti

O

Ca

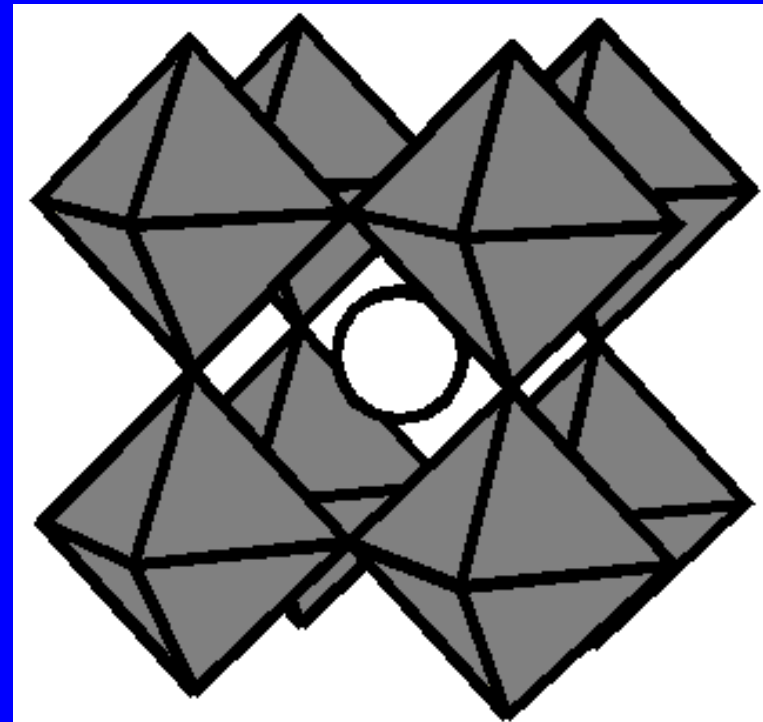
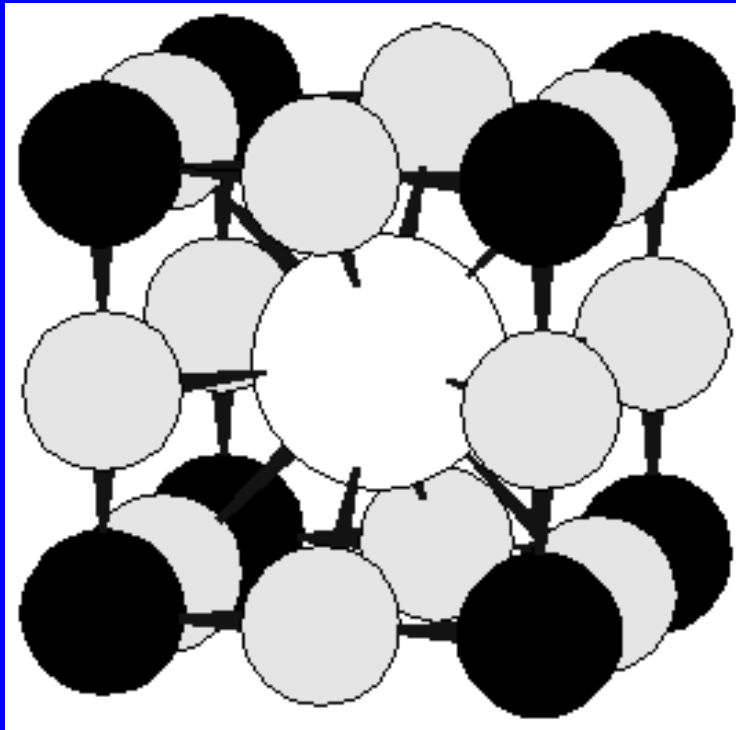


Ti

O

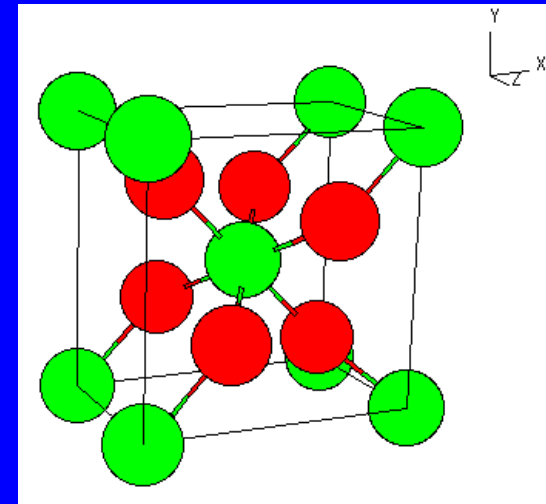
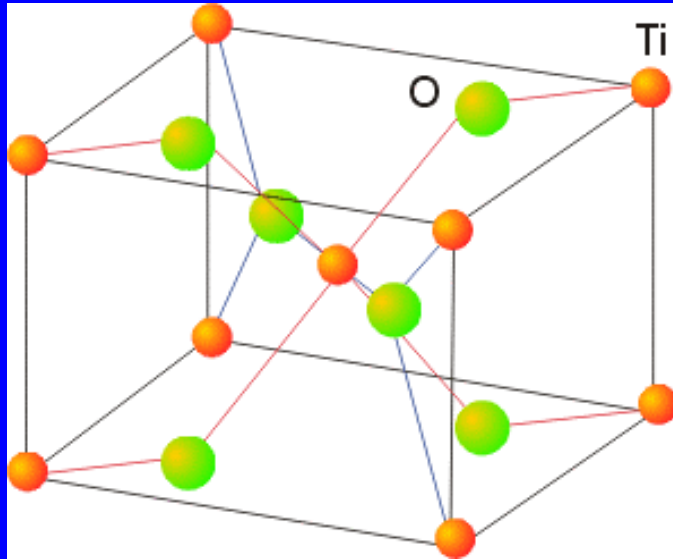
Ca

Perovskit CaTiO_3



Podobnost s CsCl

Rutil, TiO_2



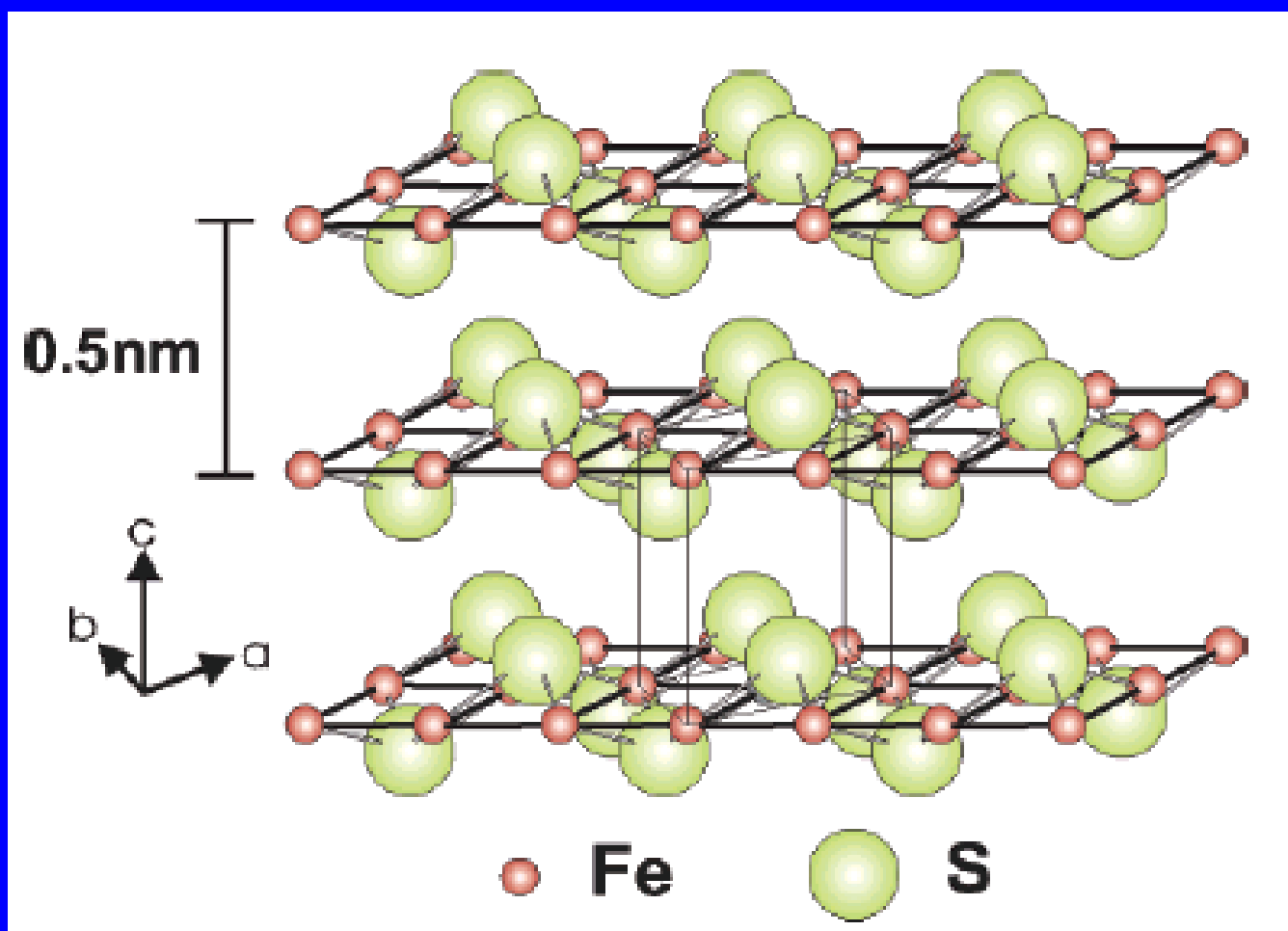
Pravidlo koordinačních čísel



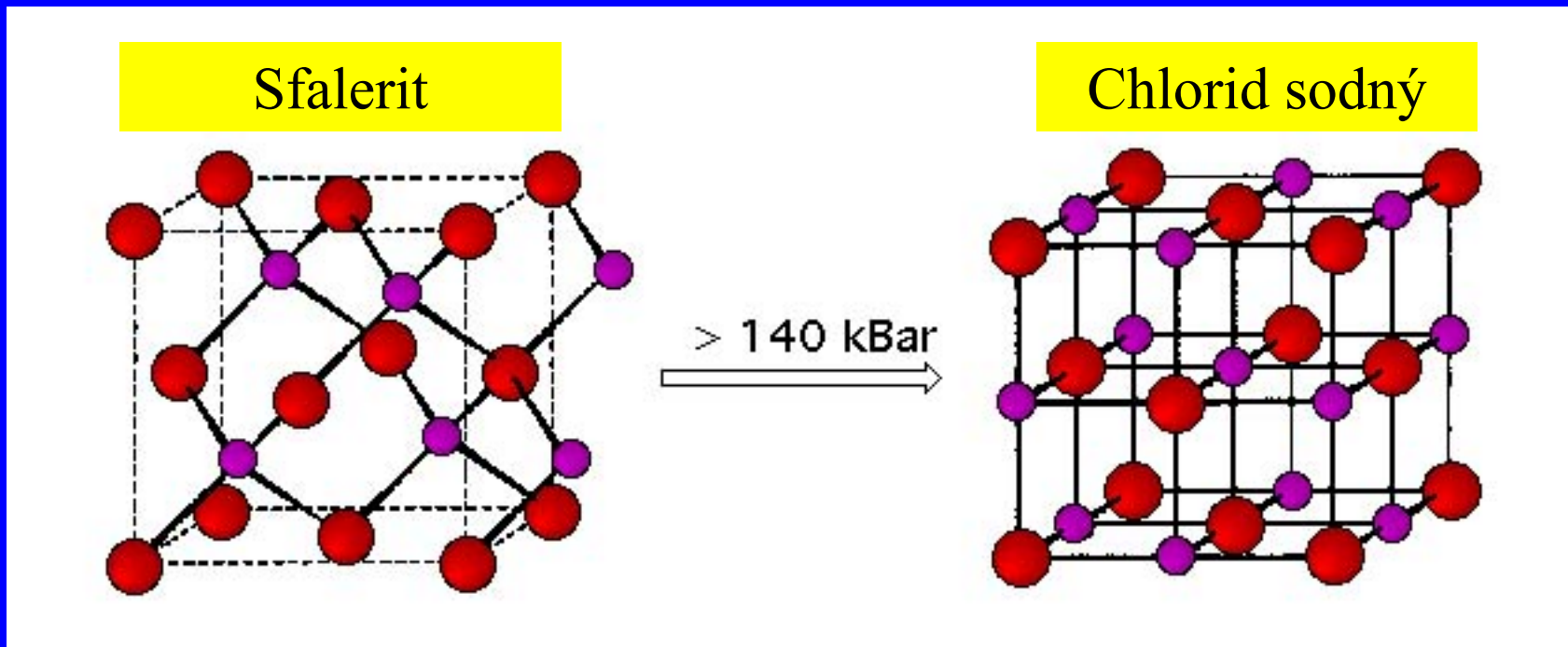
$$\text{k.č.}(A) / \text{k.č.}(B) = y / x$$

Koordinační čísla jsou v obráceném poměru stechiometrických koeficientů

Struktura mackinawitu - FeS



Fázové přeměny za zvýšeného tlaku



Důsledky zvýšení tlaku

Zvýšení koordinačního čísla

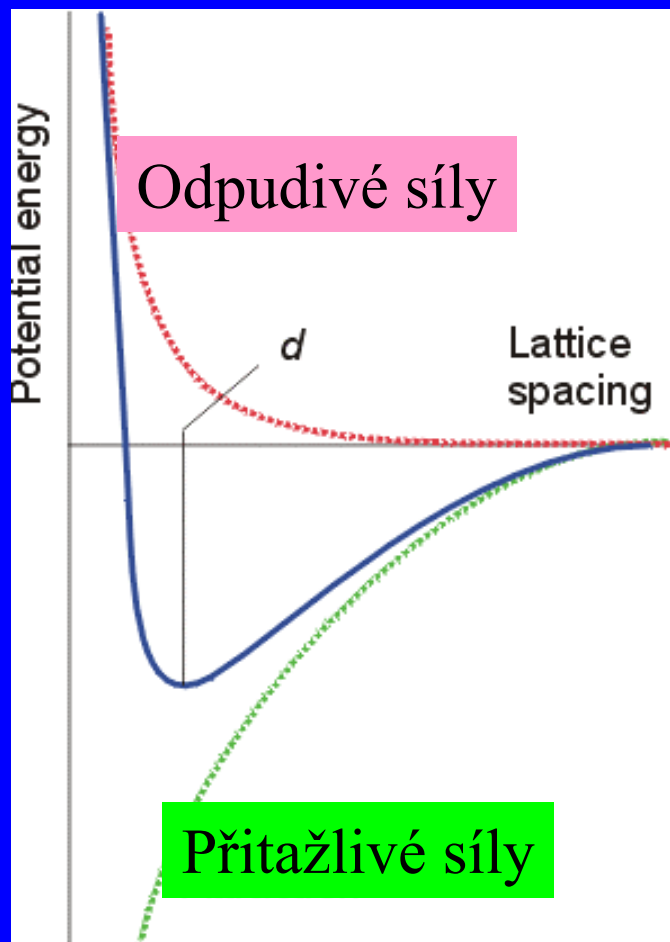
Zvýšení hustoty

Prodloužení vazebných délek

Přechod ke kovovým modifikacím 69

Mřížková energie

Mřížková energie je energie, která se uvolní při vytvoření jednoho molu pevné iontové sloučeniny z iontů v plynném stavu



$$L = E_{\text{coul}} + E_{\text{rep}}$$

Ionový pár

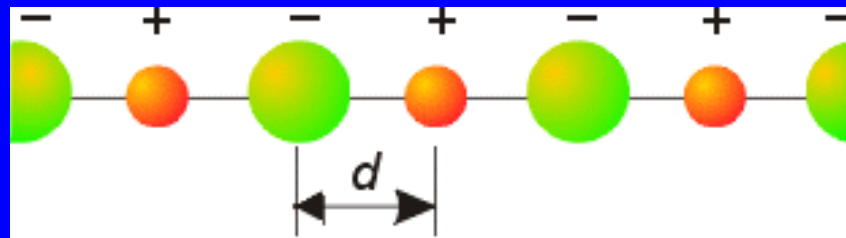
$$E_{\text{coul}} = \frac{1}{4\pi\epsilon_0} \frac{Z_A Z_B e^2}{d}$$

$$E_{\text{rep}} = \frac{B}{d^n}$$

n = Bornův exponent
(experimentálně z měření
stlačitelnosti)

Madelungova konstanta

Nutno přihlédnout ke všem interakcím v krystalové mřížce

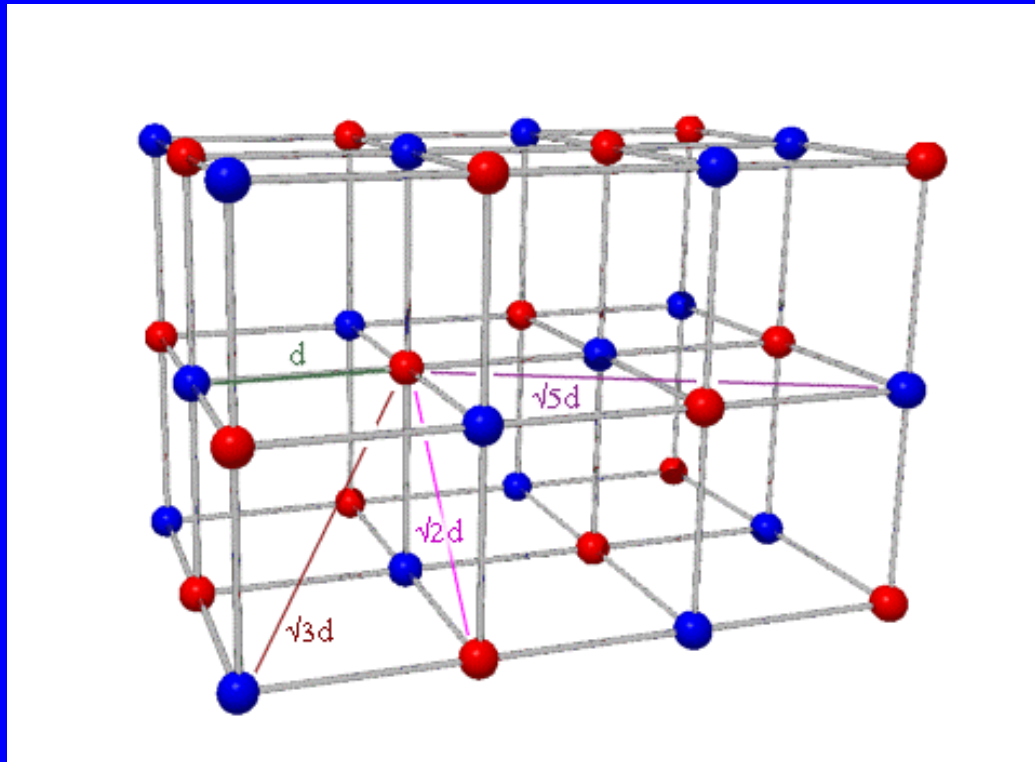


$$E_{\text{coul}} = (e^2 / 4 \pi \epsilon_0) \times (z_A z_B / d) \times [+2(1/1) - 2(1/2) + 2(1/3) - 2(1/4) + \dots]$$

$$E_{\text{coul}} = (e^2 / 4 \pi \epsilon_0) \times (z_A z_B / d) \times (2 \ln 2)$$

Madelungova konstanta M
(pro lineární uspořádání)
= součet konvergentní řady

Madelungova konstanta pro NaCl



$$E_{\text{coul}} = (e^2 / 4 \pi \epsilon_0) * (z_A z_B / d) \times [6(1/1) - 12(1/\sqrt{2}) + 8(1/\sqrt{3}) - 6(1/\sqrt{4}) + 24(1/\sqrt{5}) \dots]$$

Konvergentní řada

$$E_{\text{coul}} = (e^2 / 4 \pi \epsilon_0) \times (z_A z_B / d) \times M$$

Madelungovy konstanty pro strukturní typy

Strukturní typ	M
NaCl	1.74756
CsCl	1.76267
CaF ₂	2.519
ZnS Sfalerit	1.63805
ZnS Wurtzite	1.64132

Mřížková energie

Pro 1 mol iontů

Přitažlivá

$$E_{Coul} = N_A M \frac{Z_A Z_B e^2}{4\pi\epsilon_0 d}$$

Odpudivá

$$E_{rep} = N_A \frac{B}{d^n}$$

$$L = E_{coul} + E_{rep}$$

$$L = N_A M \frac{Z_A Z_B e^2}{4\pi\epsilon_0 d} + N_A \frac{B}{d^n}$$

Najít minimum $dL/d(d) = 0$

Mřížková energie

Born – Landeho rovnice

$$L = N_A M \frac{Z_A Z_B e^2}{4\pi\epsilon_0 d} \left(1 + \frac{1}{n} \right)$$

Born – Mayerova rovnice

$$L = N_A M \frac{Z_A Z_B e^2}{4\pi\epsilon_0 d} \left(1 - \frac{d^*}{d} \right)$$

El. konfigur.	n
He	5
Ne	7
Ar	9
Kr	10
Xe	12

$$d^* = 0.345 \text{ \AA}$$

Mřížková energie

Kapustinski

M/v je přibližně konstantní pro všechny typy struktur
 v = počet iontů ve vzorcové jednotce

M nahrazeno $0.87 v$, není nutno znát strukturu

$$L = 1210v \frac{Z_A Z_B}{d} \left(1 - \frac{0,345}{d} \right)$$

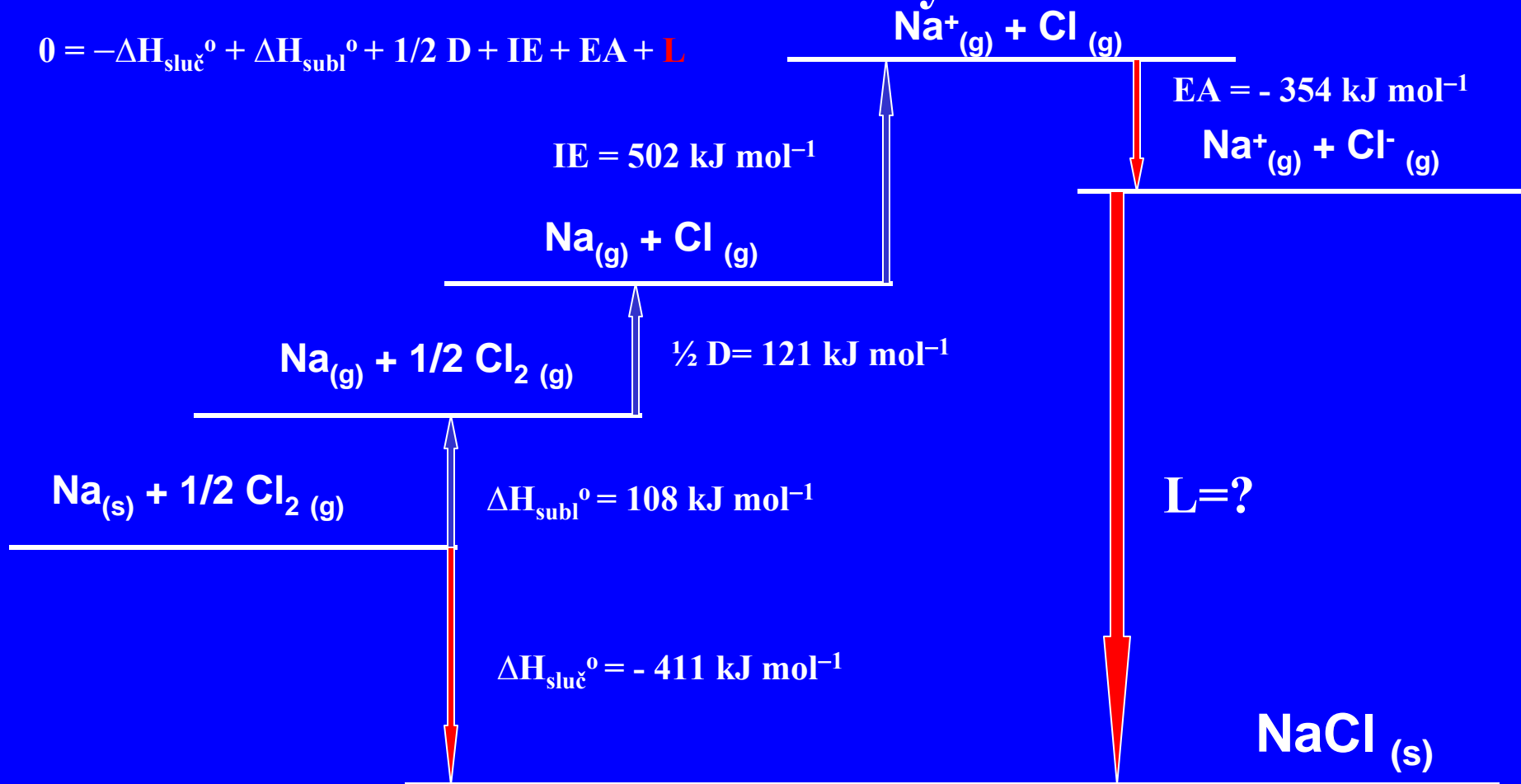
Kapustinski

struktura	M	CN	stechiom	M / ν
CsCl	1.763	(8,8)	AB	0.882
NaCl	1.748	(6,6)	AB	0.874
ZnS sfalerit	1.638	(4,4)	AB	0.819
ZnS wurtzit	1.641	(4,4)	AB	0.821
CaF ₂ fluorit	2.519	(8,4)	AB ₂	0.840
TiO ₂ rutil	2.408	(6,3)	AB ₂	0.803
CdI ₂	2.355	(6,3)	AB ₂	0.785
Al ₂ O ₃	4.172	(6,4)	A ₂ B ₃	0.834

ν = počet iontů ve vzorcové jednotce

Born-Haberův cyklus

$$0 = -\Delta H_{\text{sluč}}^{\circ} + \Delta H_{\text{subl}}^{\circ} + 1/2 D + \text{IE} + \text{EA} + L$$



$$0 = 411 + 108 + 121 + 502 + (-354) + L$$

$$L = -788 \text{ kJ mol}^{-1} \quad 78$$

Mřížková energie NaCl

Výpočtem z Born – Landeho rovnice $L = -765 \text{ kJ mol}^{-1}$
Uvažujeme jen iontový příspěvek

Měřením z Born – Haberova cyklu $L = -788 \text{ kJ mol}^{-1}$
Mřížková energie se skládá z iontového a kovalentního příspěvku