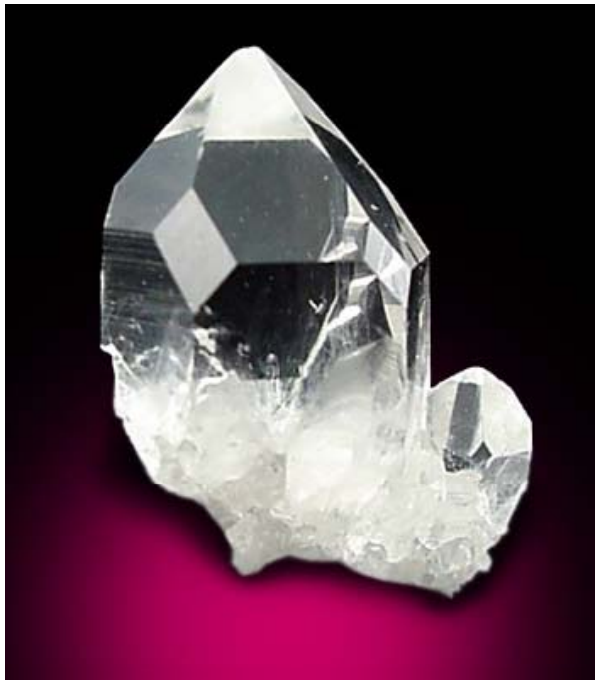
Cristalli naturali

Quarzo (SiO_2)

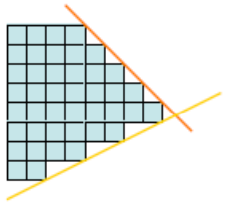


Galena (PbS)

Macroscopic regularities
(e.g. constancy of angles)

→ Classification of crystals

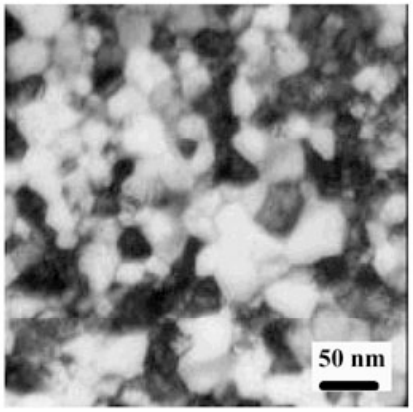
→

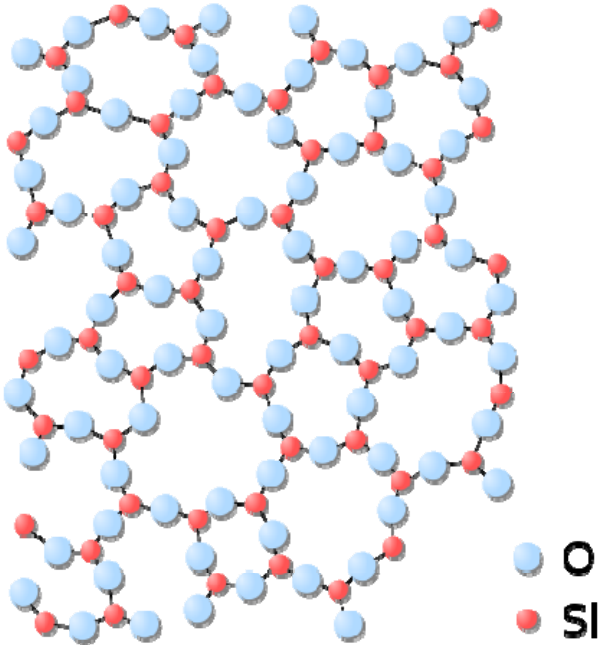


Regular packing
of microscopic structural units
R.J. Haüy (1743-1822)

Policristalli e amorfi

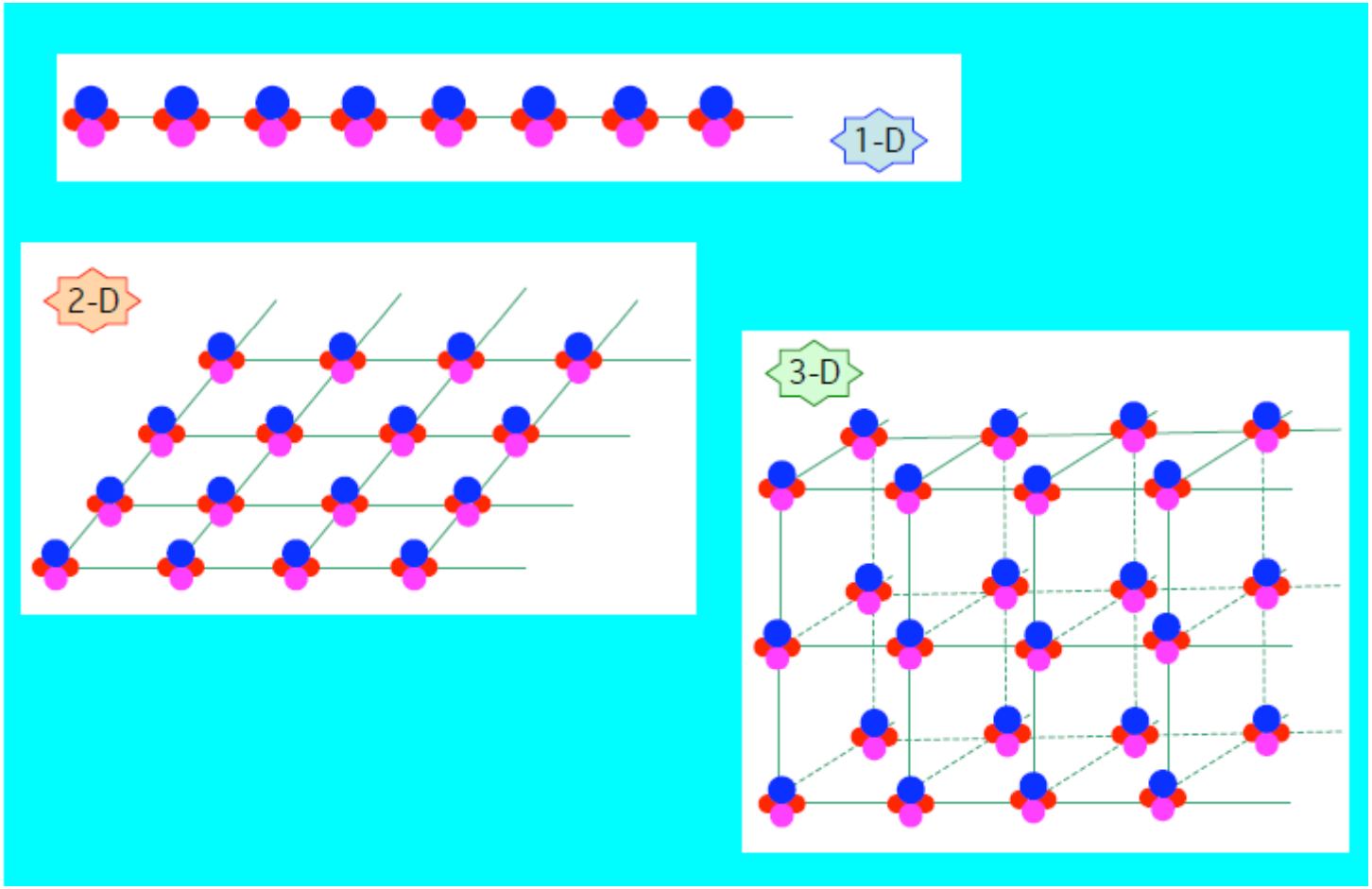
Cromo





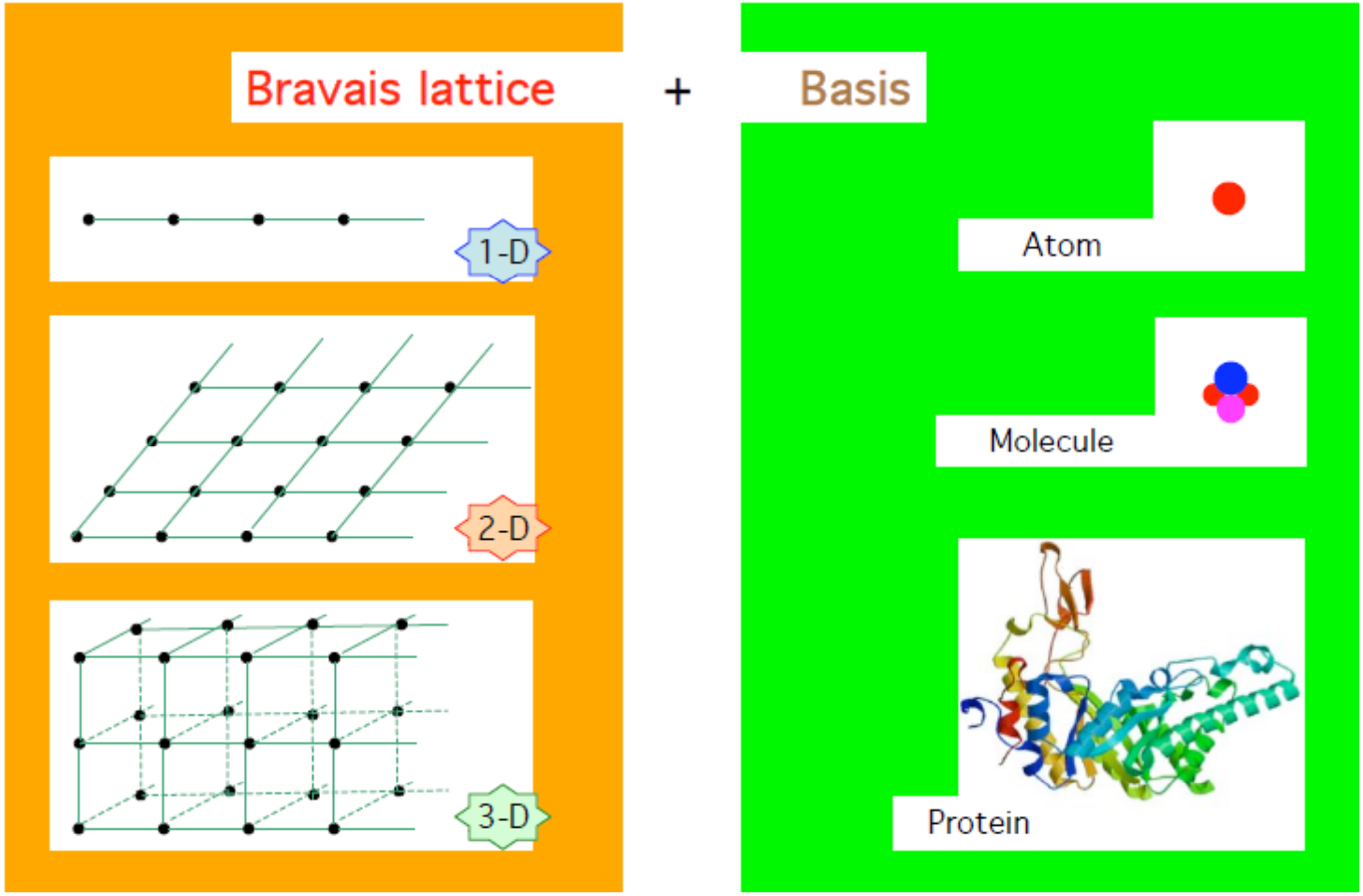
Struttura amorfa del quarzo in due dimensioni. Non esiste ordine a lungo range se si eccettua quello a primi vicini.

Struttura cristallina

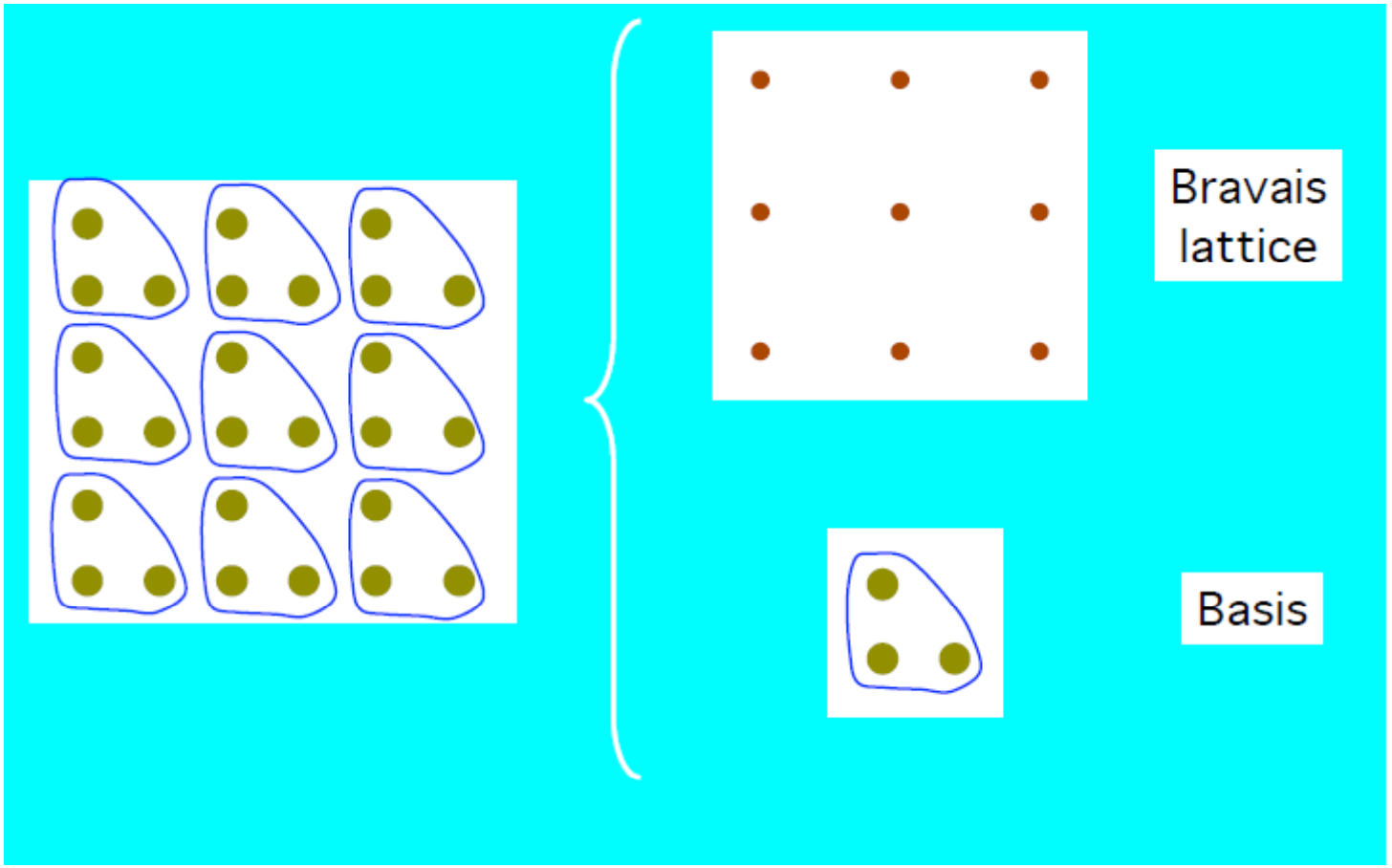


Reticolo di Bravais + base

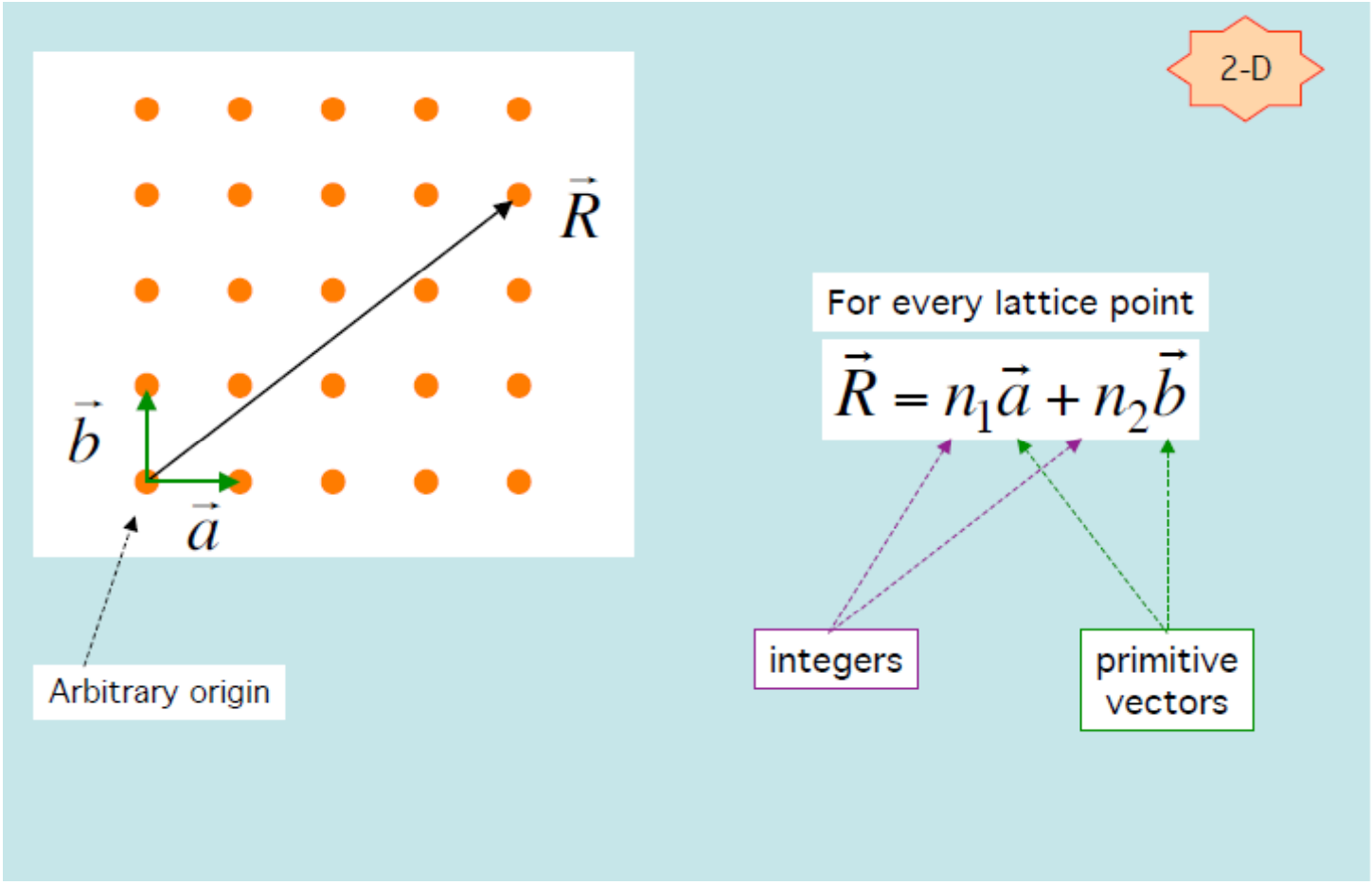
Struttura cristallina



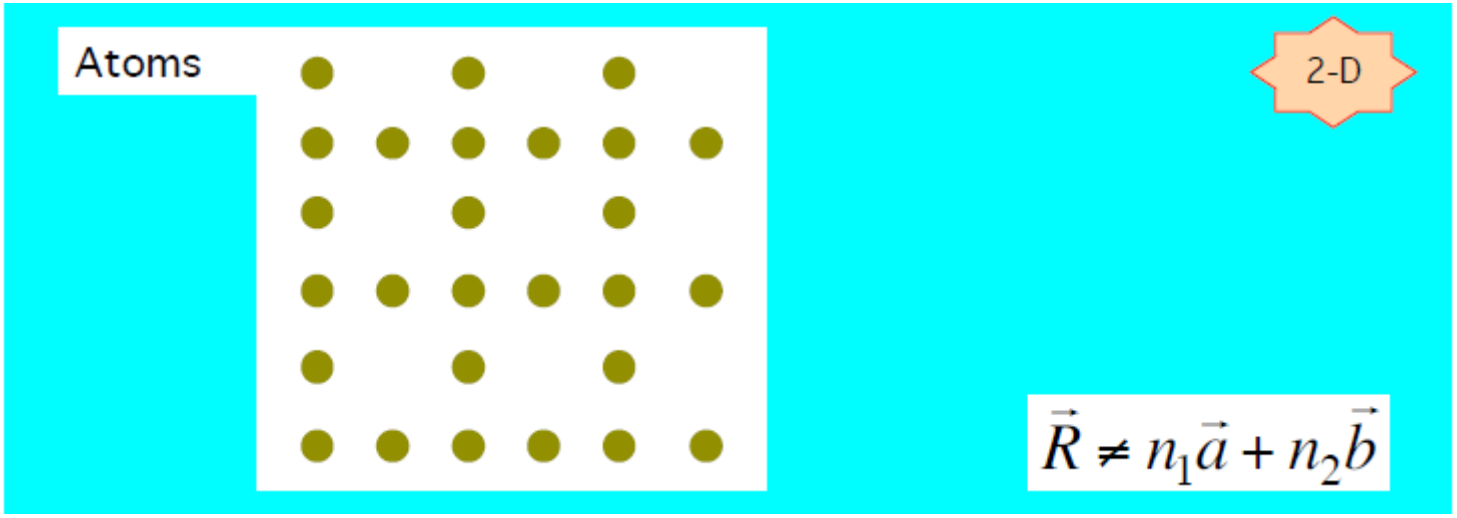
Struttura cristallina

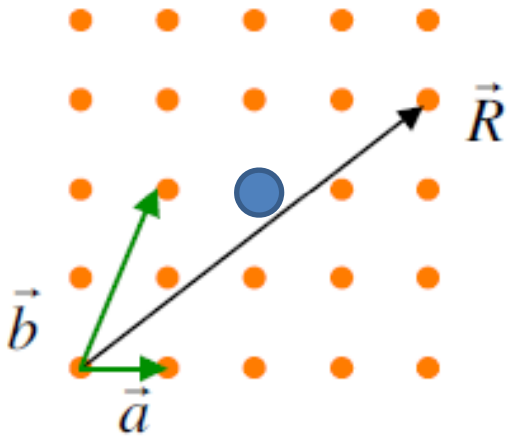


Reticoli di Bravais in 2D



Reticoli non di Bravais



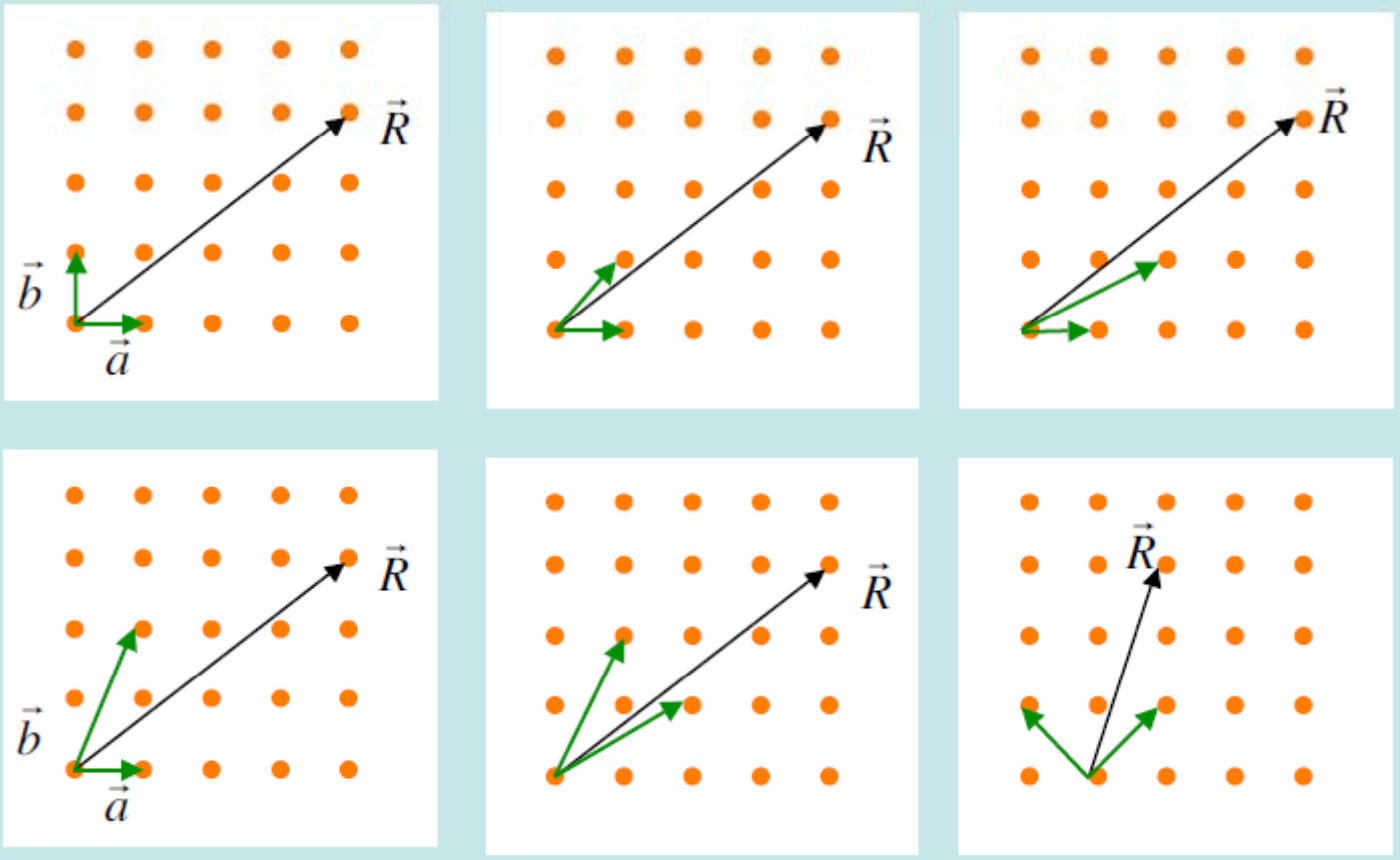


- **Un sito mancante o un atomo estraneo rompe l'invarianza traslazionale**

Vettori primitivi

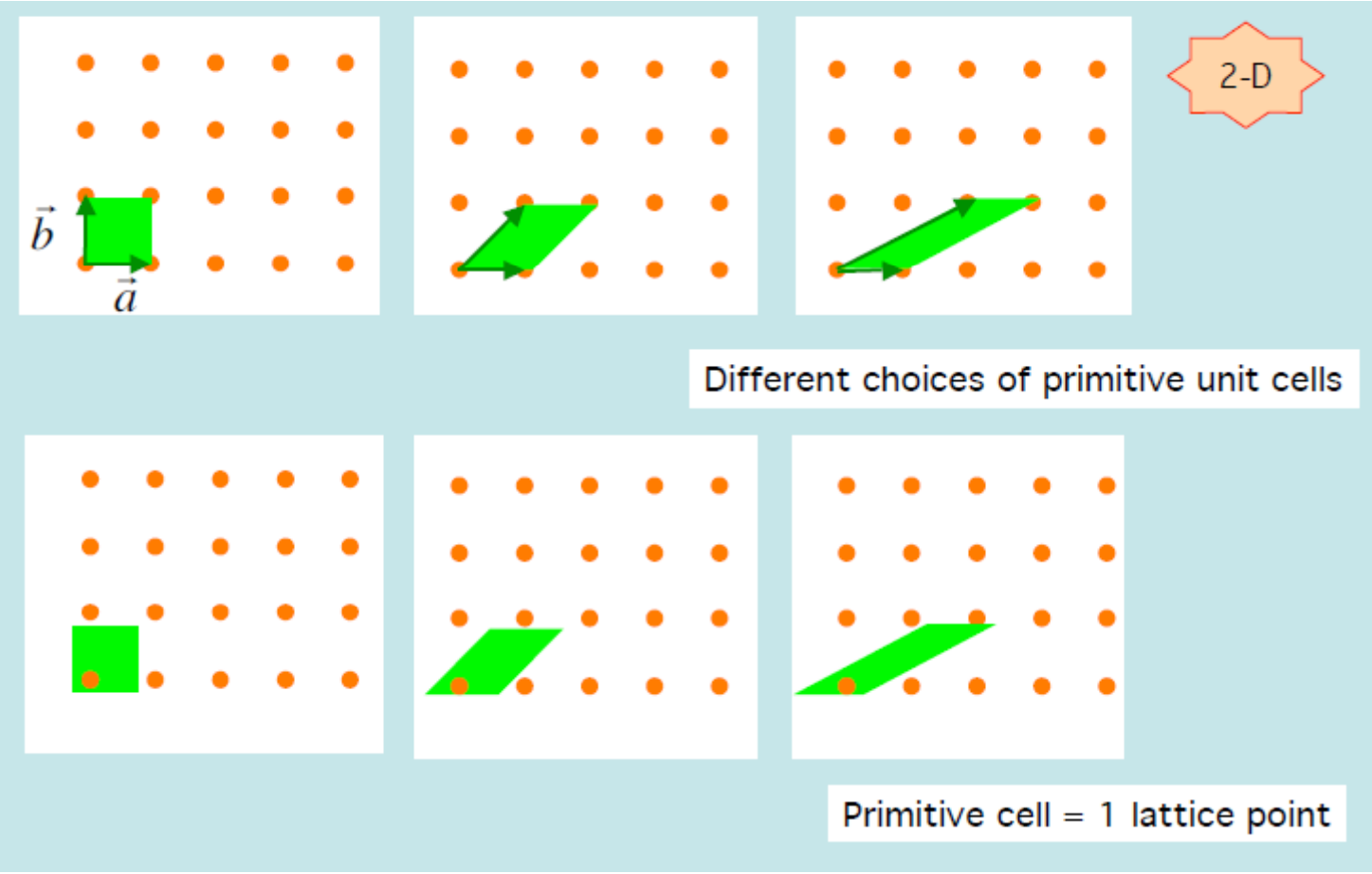
2-D

$$\vec{R} = n_1\vec{a} + n_2\vec{b}$$



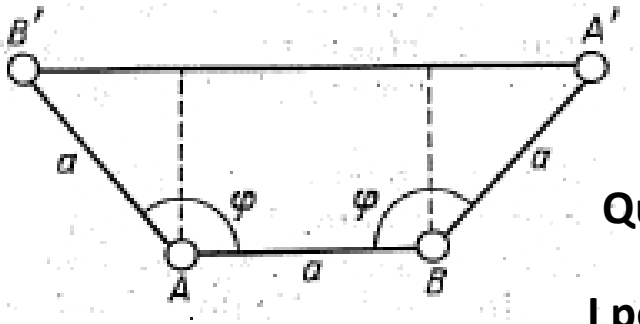
$$\vec{R} \neq n_1\vec{a} + n_2\vec{b}$$

Cella primitiva



Reticoli di Bravais

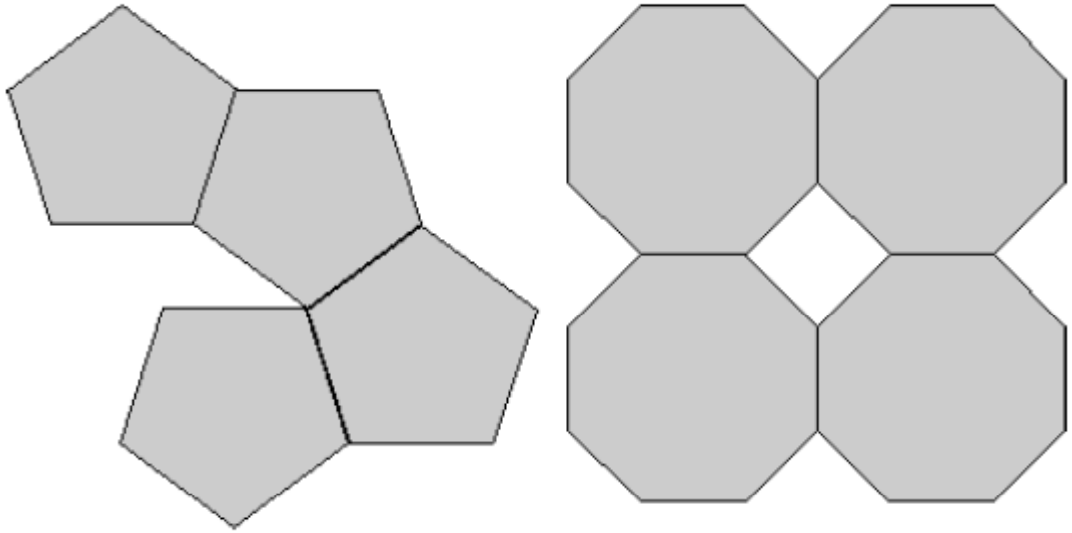
Assi di simmetria + invarianza traslazionale



$$a + 2a\sin(\varphi - \tfrac{\pi}{2}) = a - 2a\cos\varphi = \nu a \qquad \cos\varphi = \frac{1-\nu}{2}$$

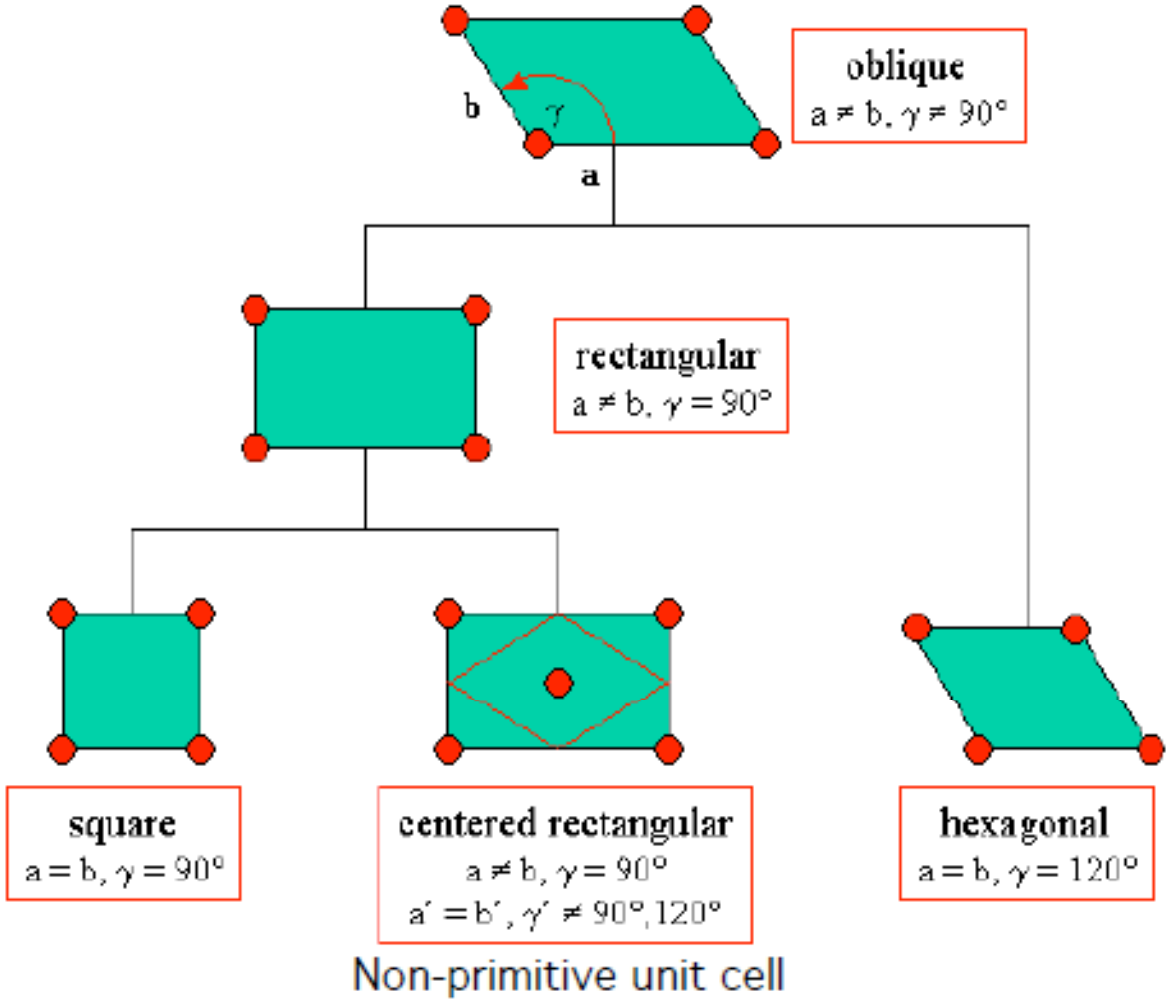
Questa equazione ha soluzioni solo per $\nu = 0,1,2,3$

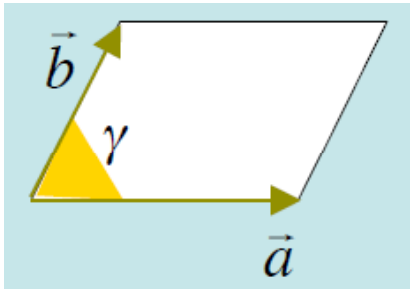
I possibili valori di ϕ sono $\varphi = \frac{2\pi}{n}$ con $n = 1,2,3,4,6$

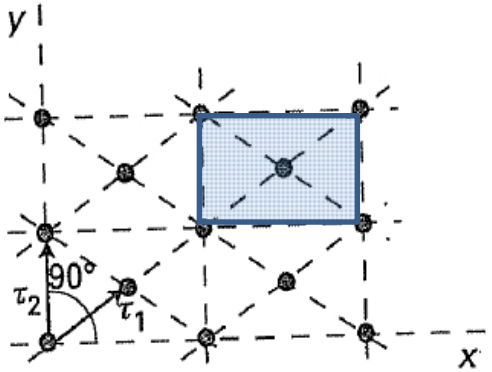


Con i pentagoni e gli ottagoni si lasciano sempre dei vuoti

Reticoli di Bravais in 2D

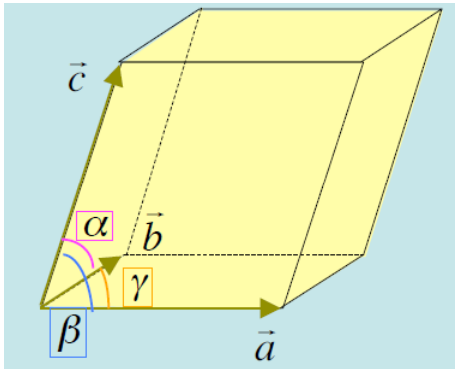




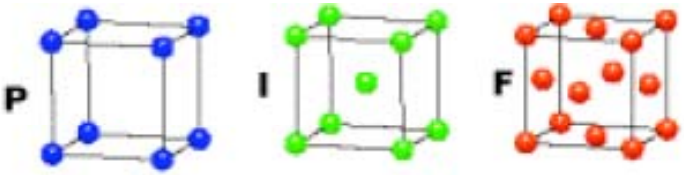


$$R = n_1\vec{a}_1 + n_2\vec{a}_2$$

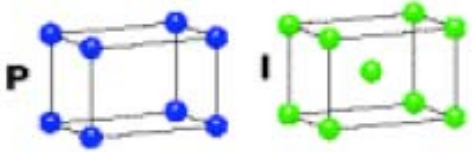
Reticoli di Bravais in 3D



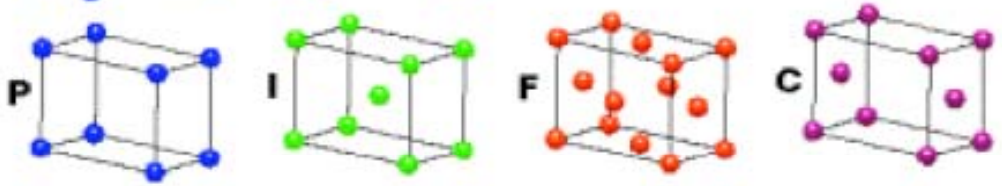
CUBIC
$a = b = c$
$\alpha = \beta = \gamma = 90°$



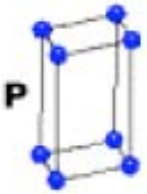
TETRAGONAL
$a = b \neq c$
$\alpha = \beta = \gamma = 90°$



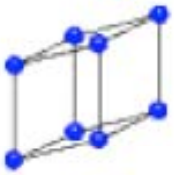
ORTHORHOMBIC
$a \neq b \neq c$
$\alpha = \beta = \gamma = 90°$



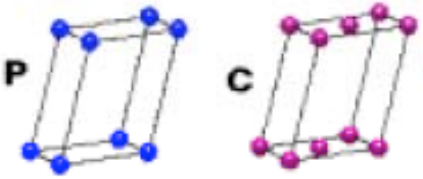
HEXAGONAL
$a = b \neq c$
$\alpha = \beta = 90°$
$\gamma = 120°$



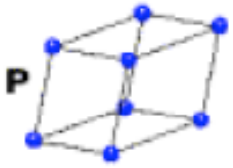
TRIGONAL
$a = b = c$
$\alpha = \beta = \gamma \neq 90°$



MONOCLINIC
$a \neq b \neq c$
$\alpha = \gamma = 90°$
$\beta \neq 120°$



TRICLINIC
$a \neq b \neq c$
$\alpha \neq \beta \neq \gamma \neq 90°$

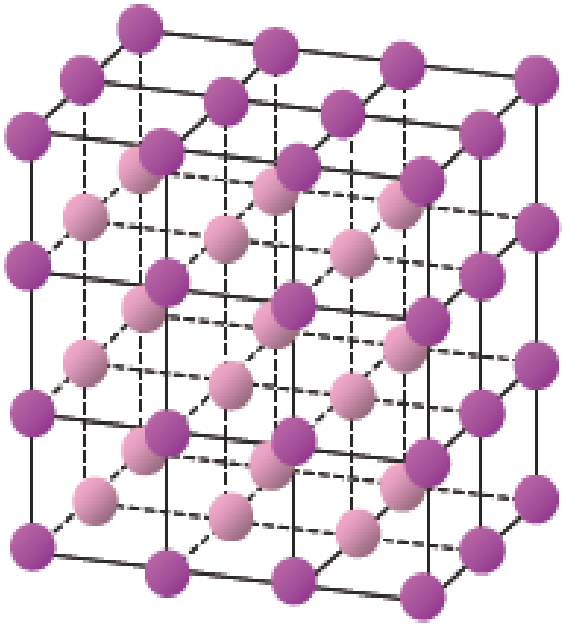


7 crystal systems + 4 unit cells (P = primitive, I = body centered, F = face centered, C = side centered) = 14 Bravais lattices

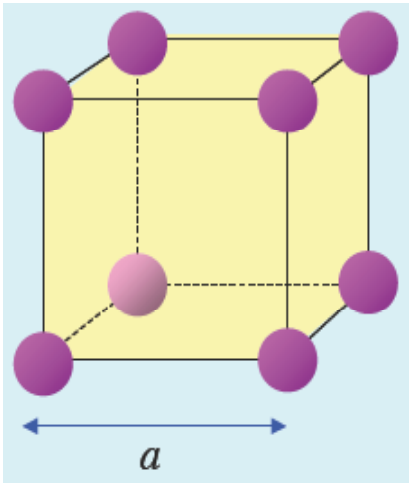
Reticoli di bravais in 3D

Cubo semplice

$$\begin{cases} \vec{a}_1 = a\hat{x} \\ \vec{a}_2 = a\hat{y} \\ \vec{a}_1 = a\hat{z} \end{cases}$$



(a)



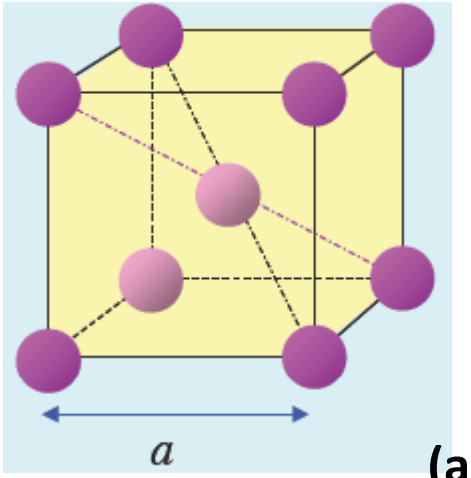
(b)

$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

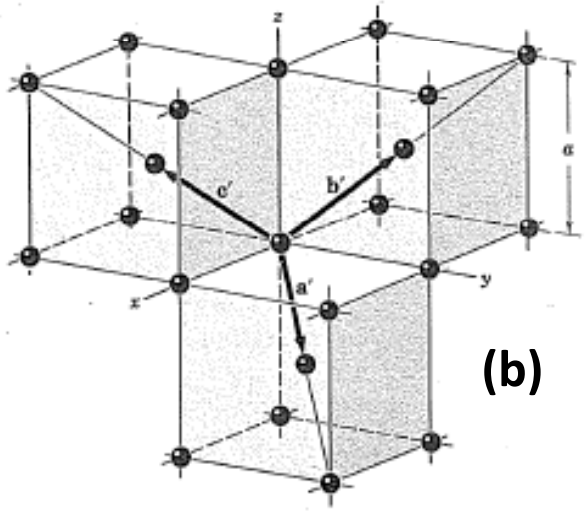
Reticoli di bravais in 3D

Cubo a corpo centrato

2 siti nella cella convenzionale



(a)



(b)

$$V_c = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = \frac{a^3}{2}$$

$$\mathbf{a}_1 = \tfrac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}})$$
$$\mathbf{a}_2 = \tfrac{a}{2}(-\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}})$$
$$\mathbf{a}_3 = \tfrac{a}{2}(\hat{\mathbf{x}} - \hat{\mathbf{y}} + \hat{\mathbf{z}})$$

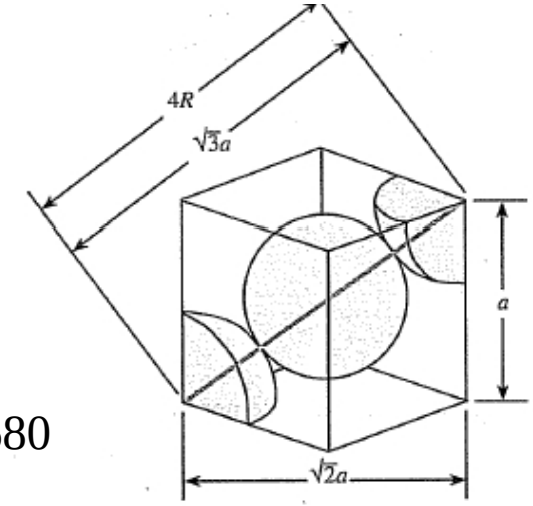
8 primi vicini nelle posizioni $\left(\pm\frac{a}{2},\pm\frac{a}{2},\pm\frac{a}{2}\right)$

6 secondi vicini nelle posizioni $(\pm a,0,0),(0,\pm a,0),(0,0,\pm a)$

Elemento	a (Å)	Elemento	a (Å)
Li	3.49	Cr	2.88
Na	4.32	Nb	3.300
K	5.25	Mo	3.147
Rb	5.60	V	3.024
Cs	6.07	W	3.165

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

$$F = \frac{4\pi R^3/3}{a^3}2 = 0.680$$

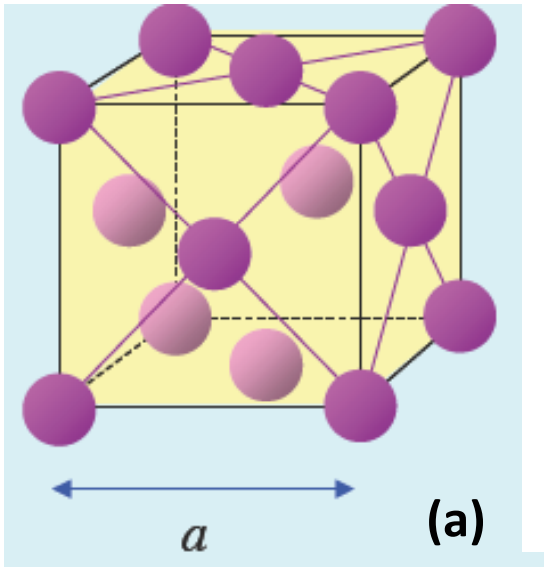


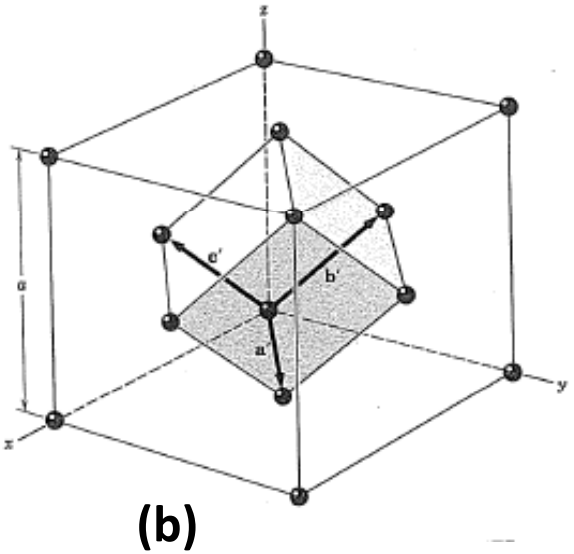
Reticoli di bravais in 3D

Cubo a facce centrate

4 siti nella cella convenzionale

$$V_c = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = \frac{a^3}{4}$$





12 primi vicini nelle posizioni

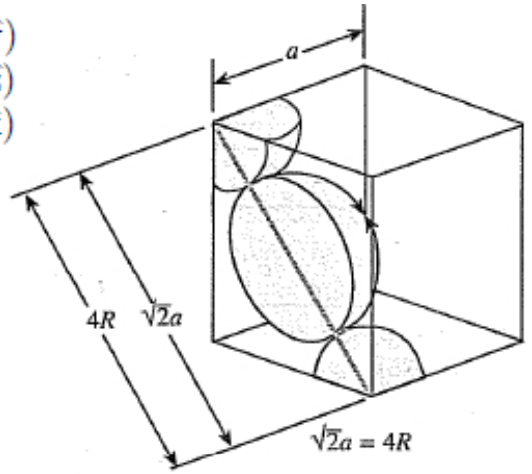
$$\left(\pm\frac{a}{2},\pm\frac{a}{2},0\right),\left(\pm\frac{a}{2},0,\pm\frac{a}{2}\right),\left(0,\pm\frac{a}{2},\pm\frac{a}{2}\right)$$

6 secondi vicini nelle posizioni

$$(\pm a,0,0),(0,\pm a,0),(0,0,\pm a)$$

Elemento	a (Å)	Elemento	a (Å)
Ne	4.439	Ag	4.086
Ar	5.256	Au	4.078
Kr	5.721	Co	3.548
Xe	6.197	Ni	3.524
Al	4.050	Pd	3.89
Cu	3.615	Pt	3.923

$$\mathbf{a}_1 = \tfrac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}})$$
$$\mathbf{a}_2 = \tfrac{a}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}})$$
$$\mathbf{a}_3 = \tfrac{a}{2}(\hat{\mathbf{z}} + \hat{\mathbf{x}})$$

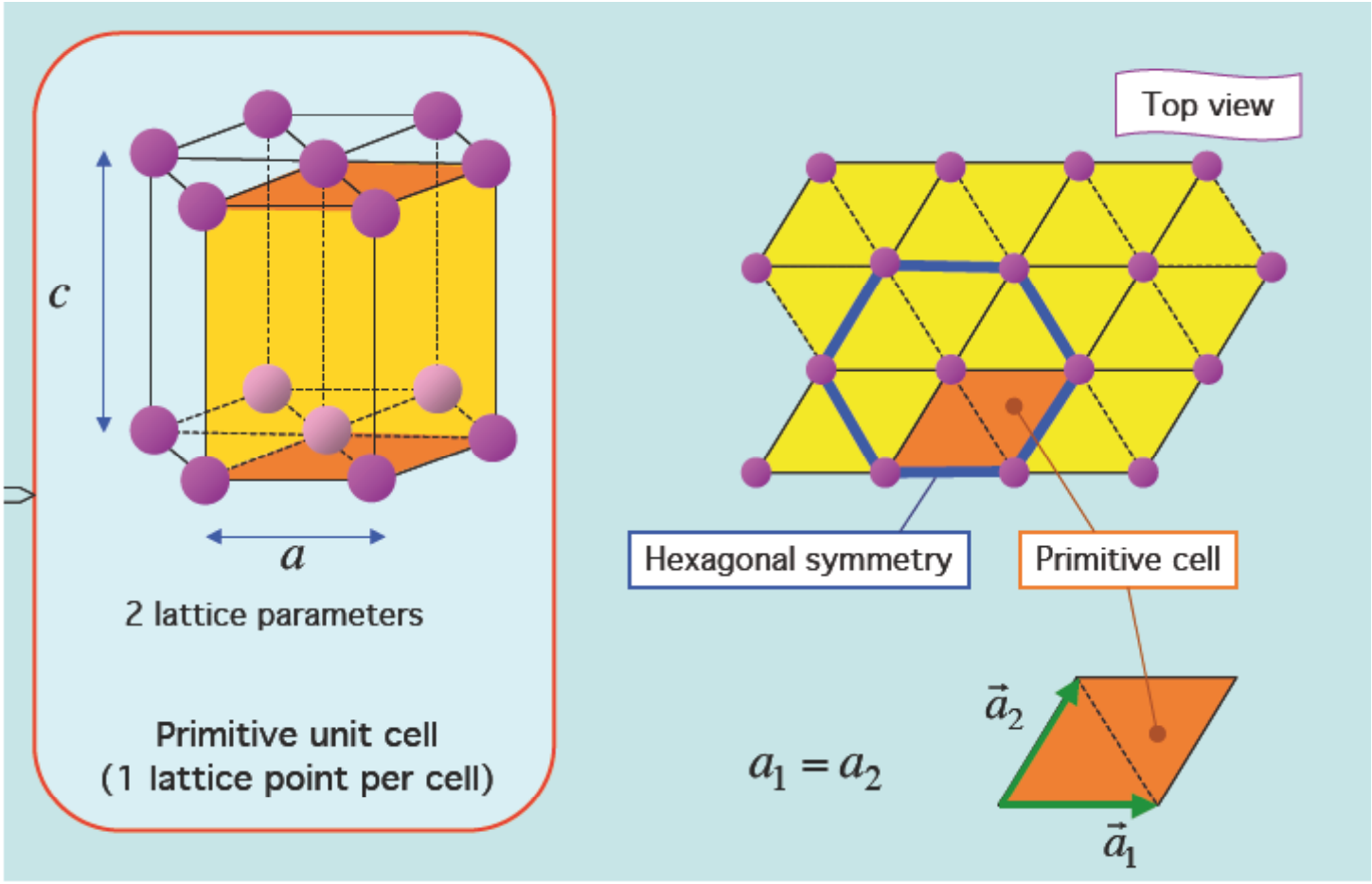


$$R = \frac{a}{4}\sqrt{2}$$

$$F = \frac{4\pi R^3/3}{a^3}4 = 0.740$$

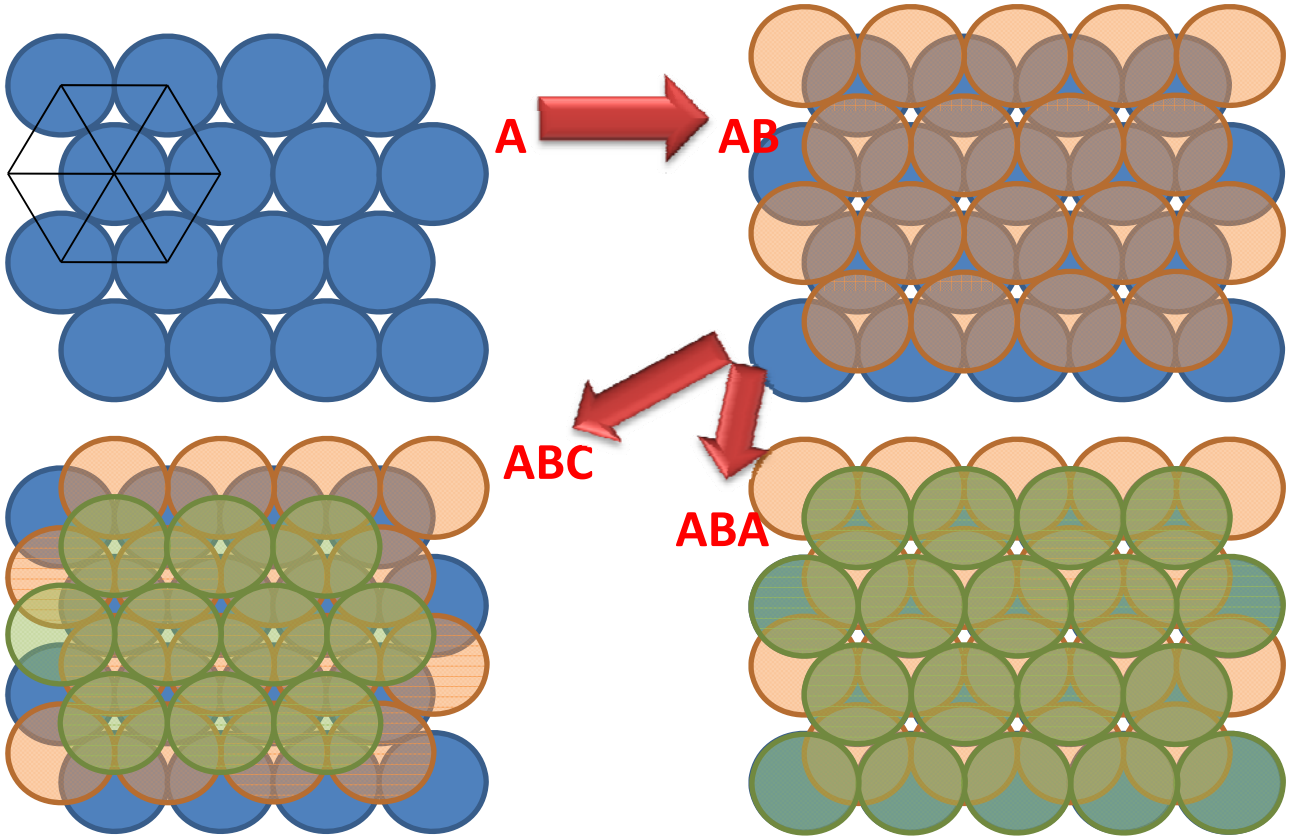
Reticoli di bravais in 3D

Esagonale semplice



3 siti per cella convenzionale

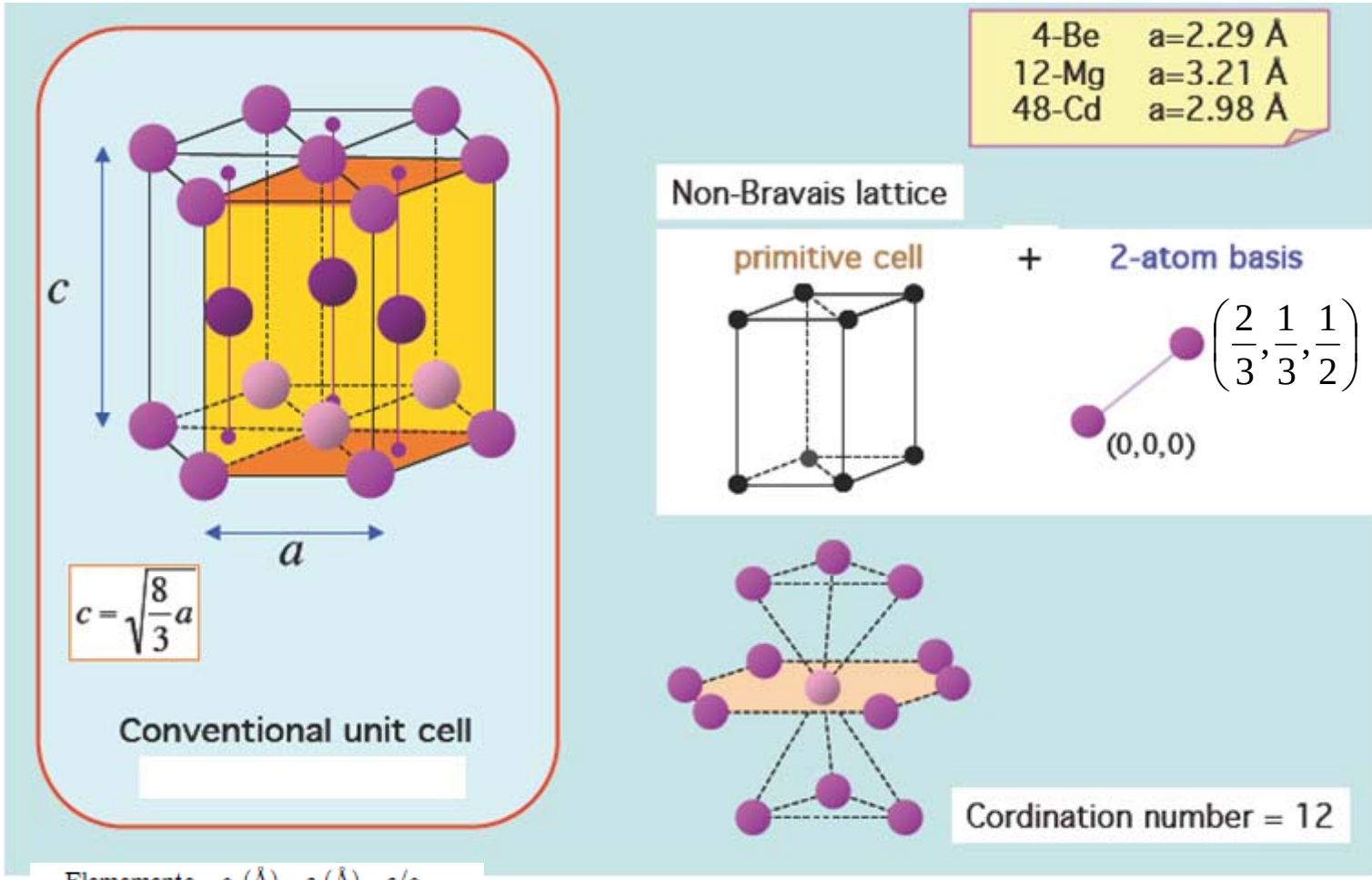
Strutture cristalline compatte



Cubo a facce centrate

Esagonale compatto

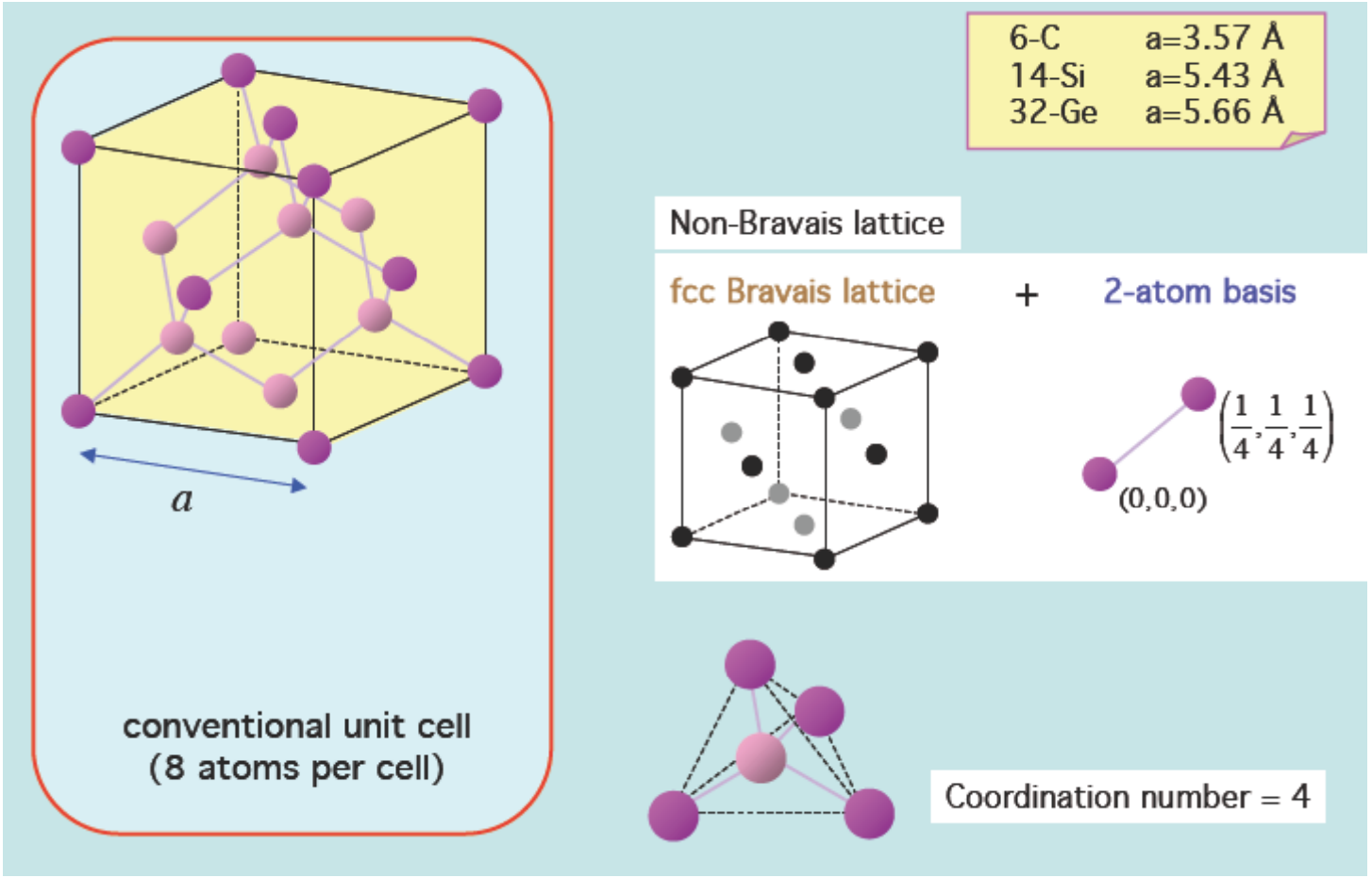
Esagonale compatto



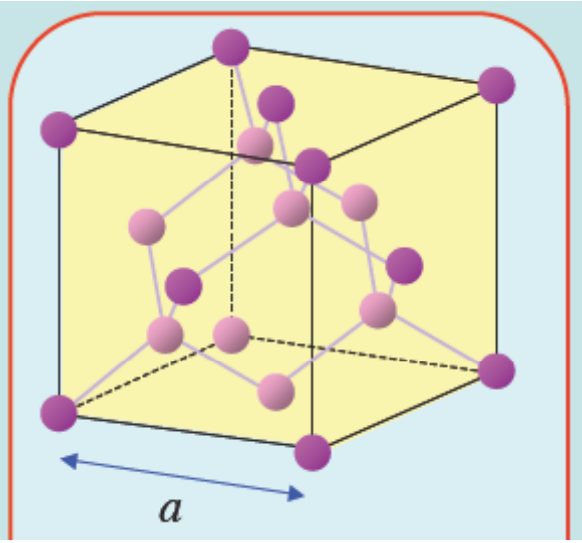
Elememento	a (Å)	c (Å)	c/a
He	3.57	5.83	1.6331
Be	2.287	3.583	1.5667
Mg	3.209	5.210	1.6235
Cs (β)	3.98	6.52	1.6382
Sr (β)	4.32	7.06	1.6343
Na	3.767	6.154	1.6336
Ni	2.65	4.33	1.6340
Ti	2.95	4.69	1.5898
Y	3.647	5.731	1.5714
Zn	2.665	4.947	1.8562

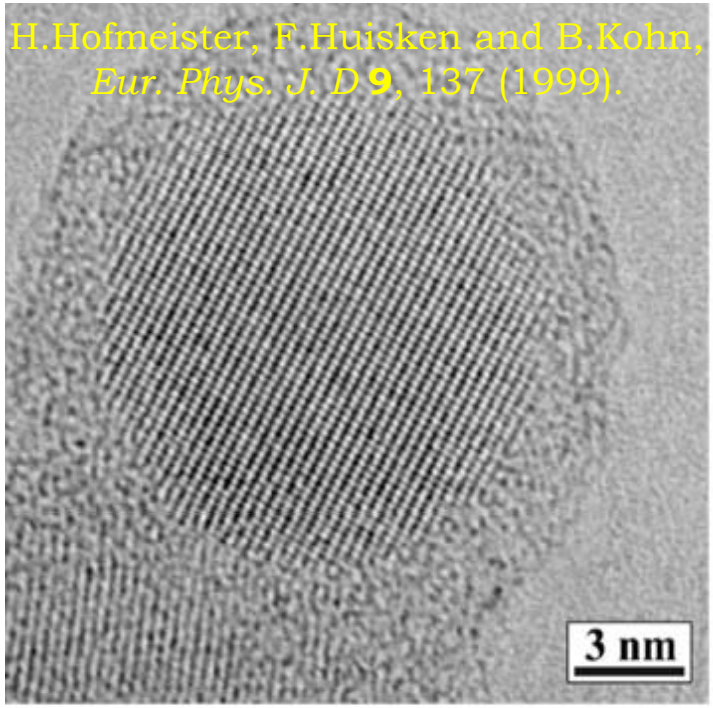
6 atomi per cella convenzionale

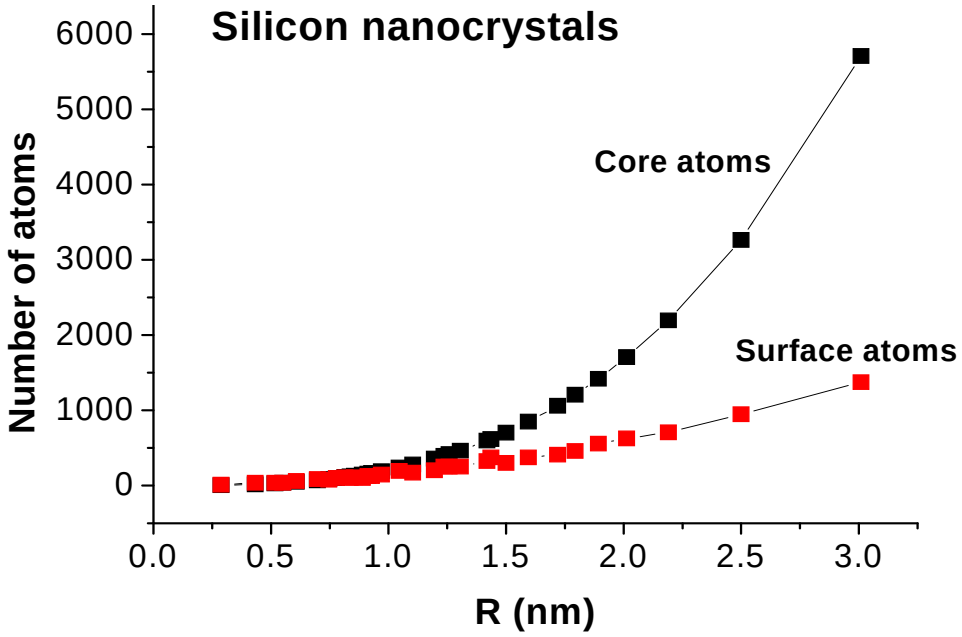
Struttura del diamante

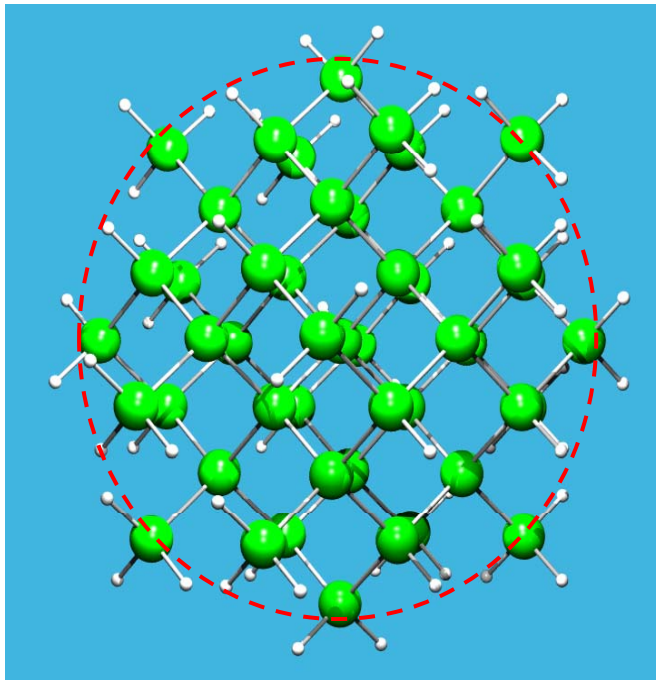


Nanocristalli di silicio

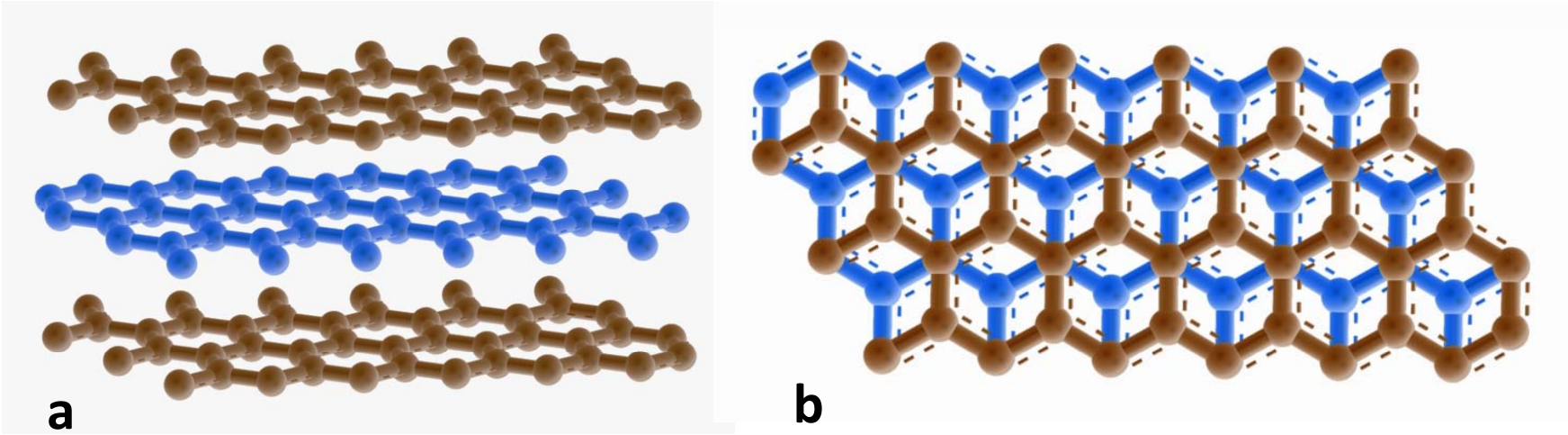




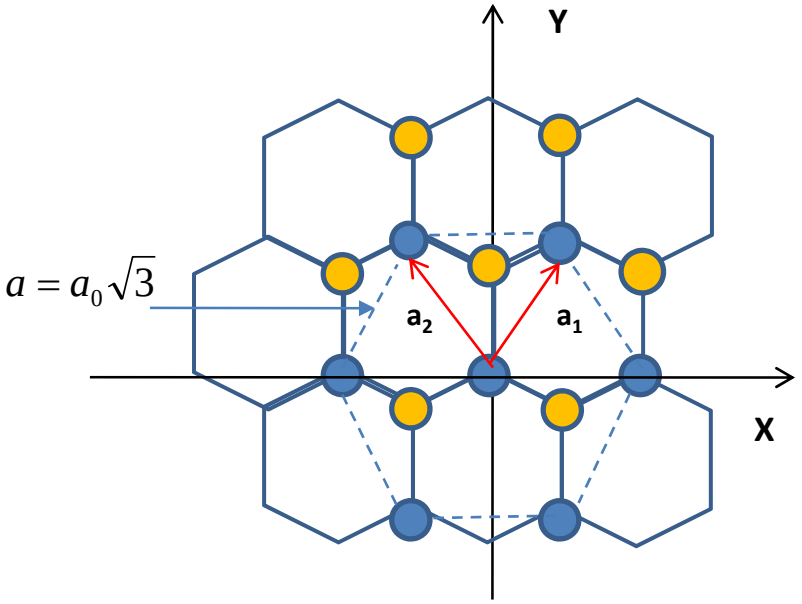




Struttura della grafite



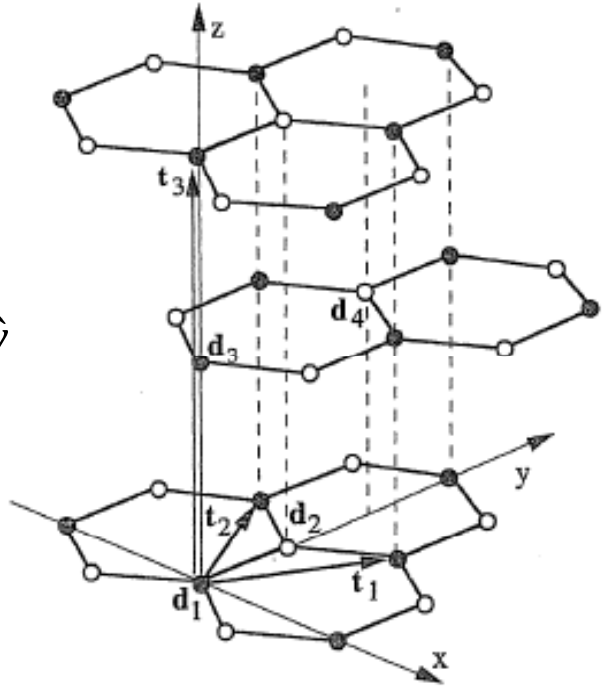
Esagonale + base di 4 atomi



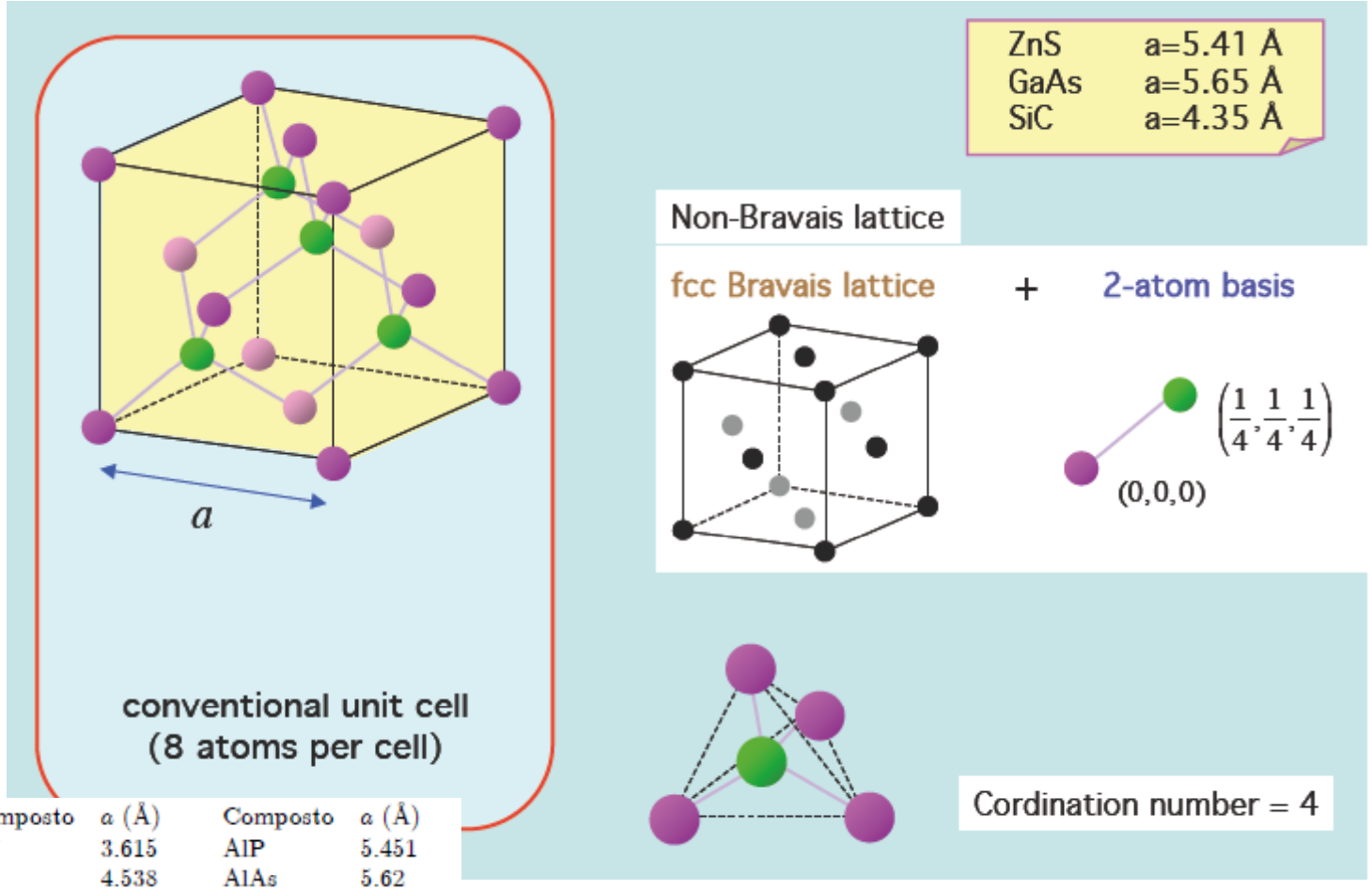
$$\vec{a}_1 = \frac{a}{2}\hat{x} + \frac{a\sqrt{3}}{2}\hat{y}$$

$$\vec{a}_2 = -\frac{a}{2}\hat{x} + \frac{a\sqrt{3}}{2}\hat{y}$$

$$a_0 = 1.42$$



Zincoblenda (ZnS)



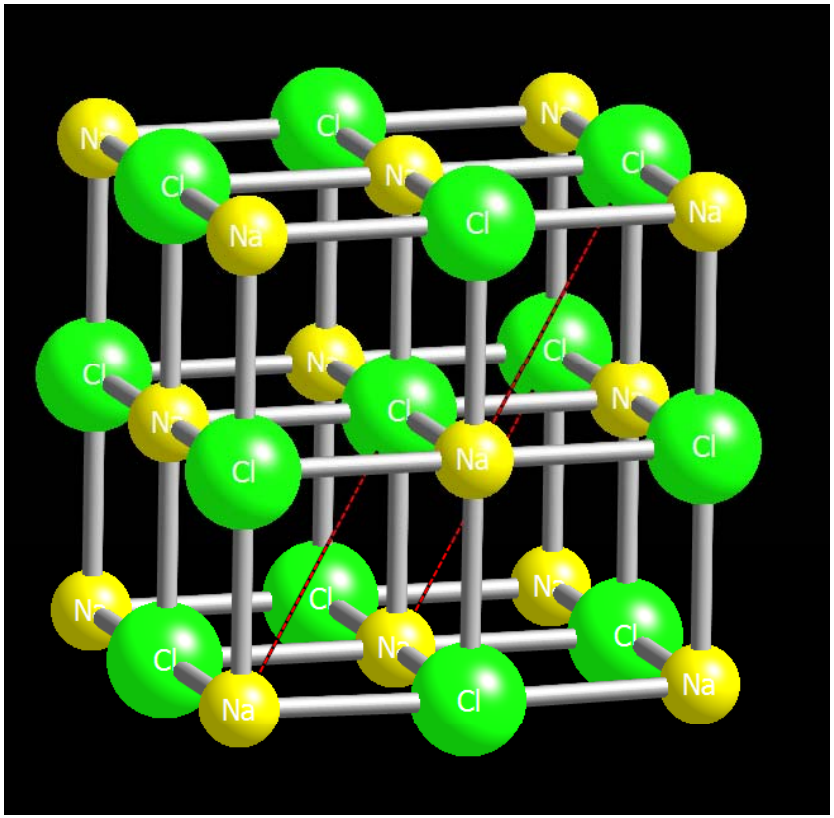
Composto	a (Å)	Composto	a (Å)
BN	3.615	AlP	5.451
BP	4.538	AlAs	5.62
BAs	4.777	AlSb	6.1347
GaP	5.4505	InP	5.8687
GaAs	5.6537	InAs	6.036
GaSb	6.118	InSb	6.4782
CdS	5.818	HgS	5.8517
CdTe	6.480	HgTe	6.429
CuF	4.255	ZnS	5.4093
CuCl	5.4057	ZnSe	5.6676
CuBr	5.6905	ZnTe	6.089
CuI	6.0427		

Cloruro di sodio

Cubo a facce centrate + Base

Na^+ (0,0,0)

Cl^- (1/2,1/2,1/2)



Composto	a (Å)	Composto	a (Å)	Composto	a (Å)
LiH	4.085	AgCl	5.547	RbH	6.037
LiF	4.027	AgBr	5.775	RbF	5.64
LiCl	5.120	MgO	4.211	RbCl	6.58
LiBr	5.501	CaO	4.81	RbBr	6.85
LiI	6.000	CdO	4.695	RbI	7.342
KH	5.70	NaH	4.88	MnO	4.445
KF	5.347	NaF	4.620	FeO	4.31
KCl	6.293	NaCl	5.63	NiO	4.168
KBr	6.60	NaBr	5.973	TiO	4.177
AgF	4.92	NaI	6.473	MnS	5.224

Cloruro di cesio (ClCs)

Cubo Semplice + base

Cs^+ (0,0,0)

Cl^- (1/2,1/2,1/2)

Composto	a (Å)	Composto	a (Å)
CsBr	4.286	TlCl	3.834
CsI	4.567	TlBr	3.97
RbCl	3.74	TlI	4.198
ThTe	3.827