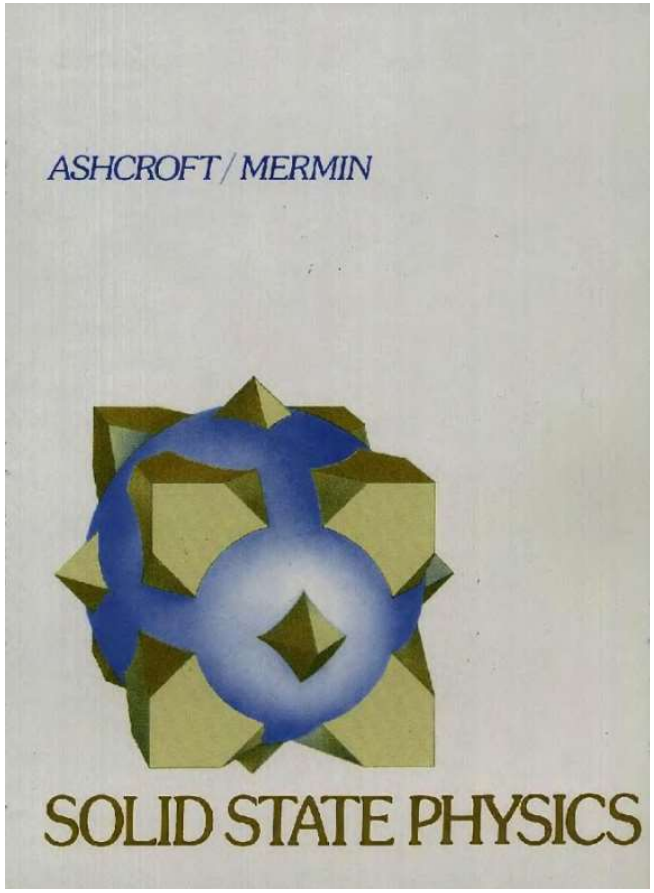
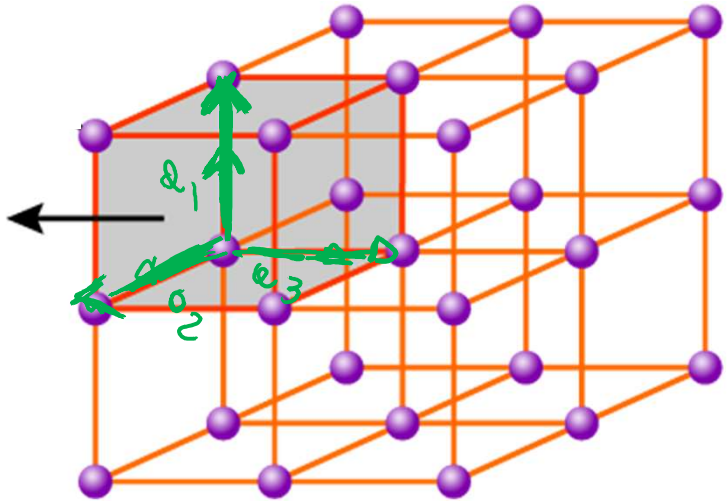


Capitoli 4 e 5

Il reticolo cristallino

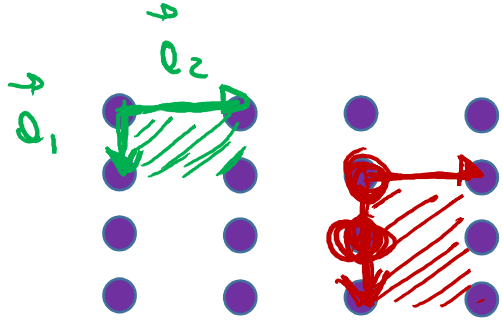


cella unitaria

$\vec{a}_1, \vec{a}_2, a_3$ vettori della cella

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

3D

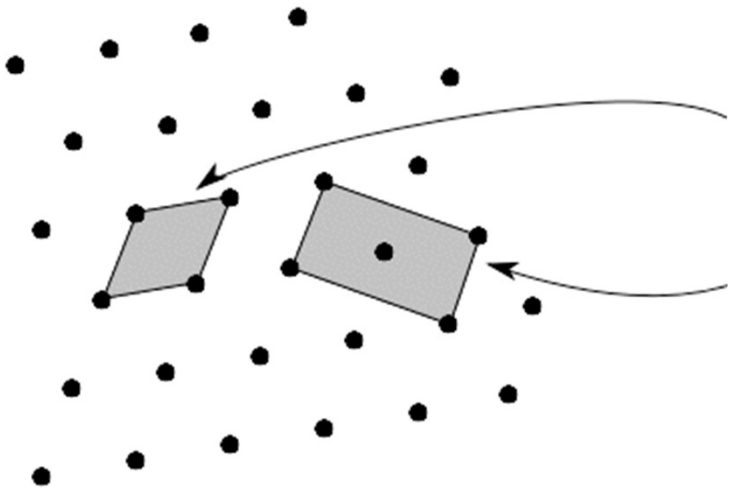


base della cella

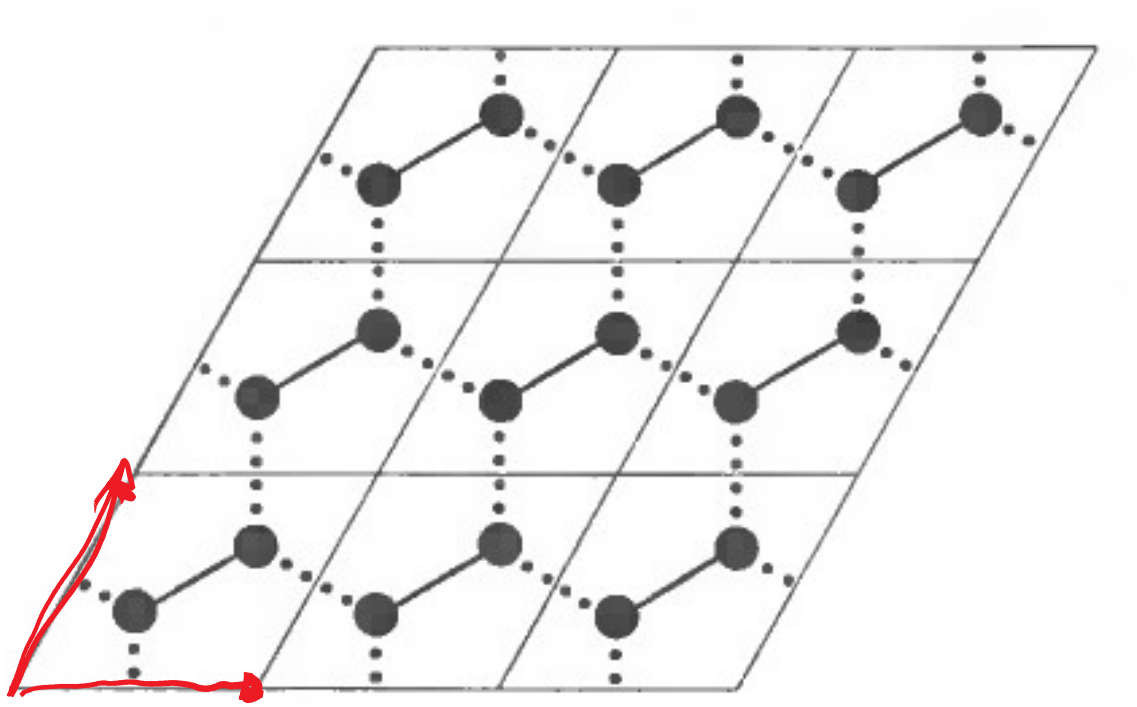
$(0,0), \left(\frac{1}{2}, 0\right)$

2D

CELLA PRIMITIVA VS UNITARIA

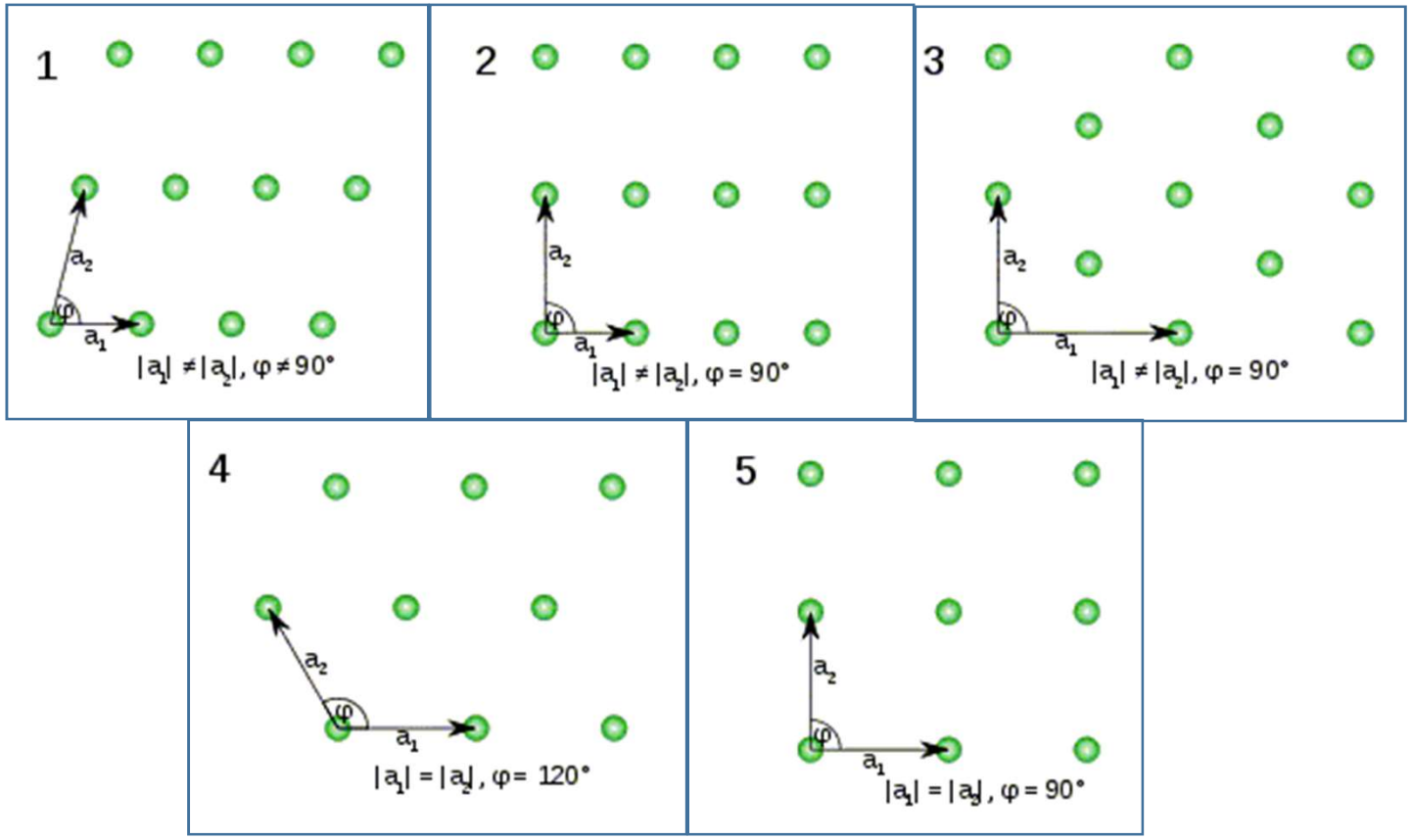

primitiva
unitaria
"convenzionale"

RETICOLO CON CELLA

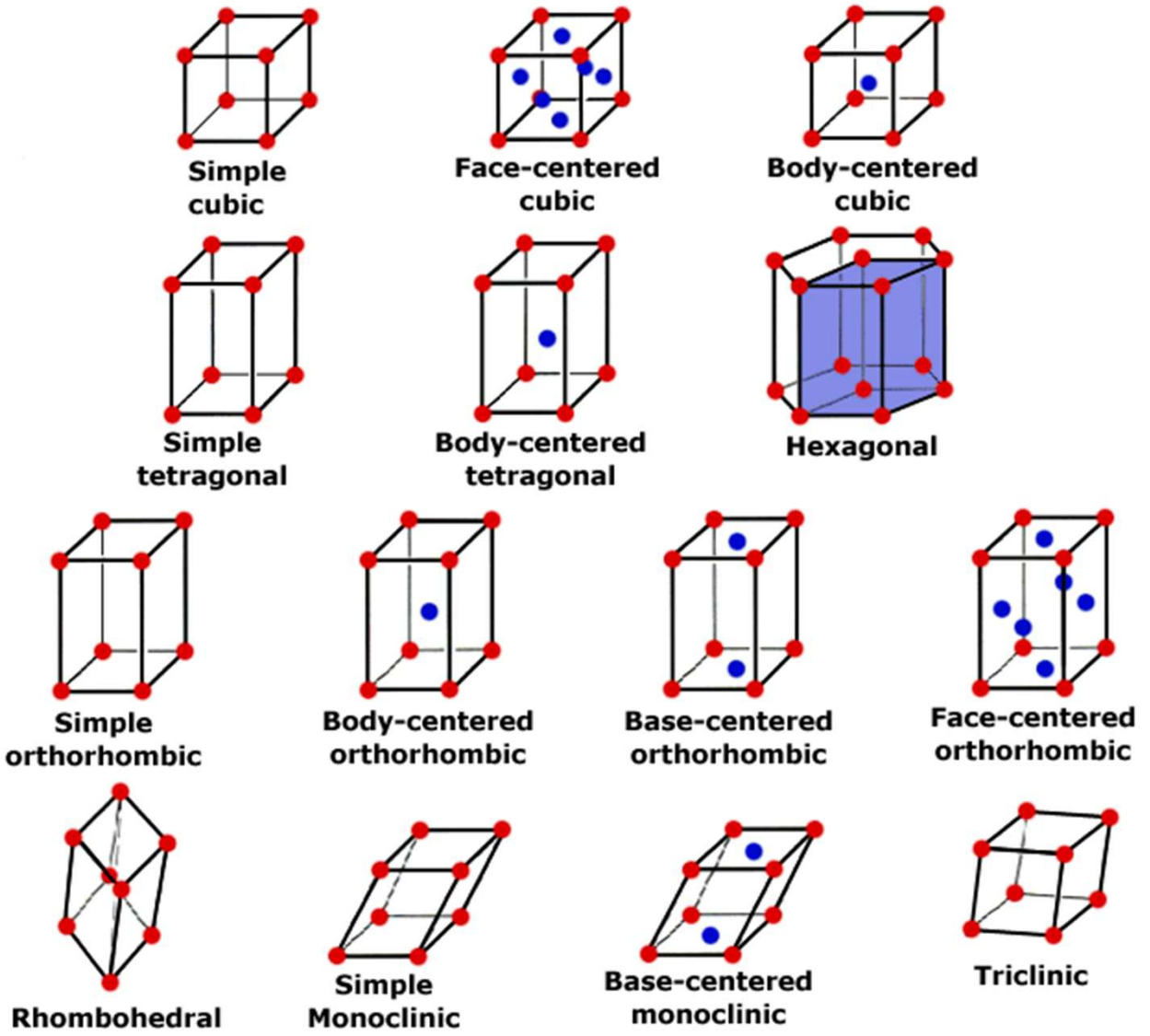


RETICOLO
honeycomb

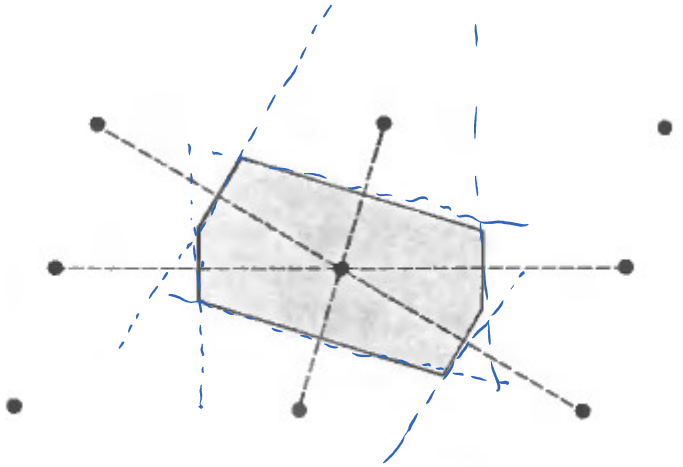
Reticoli di Bravais 2D

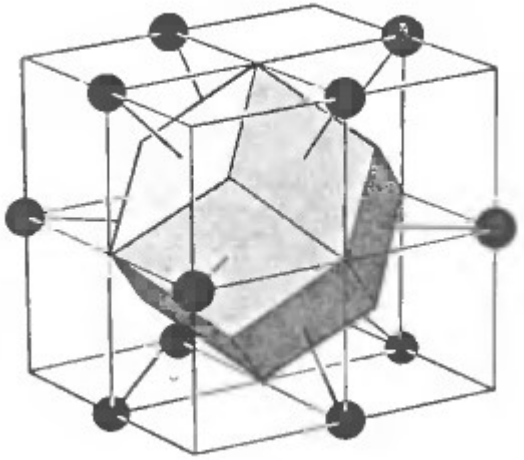


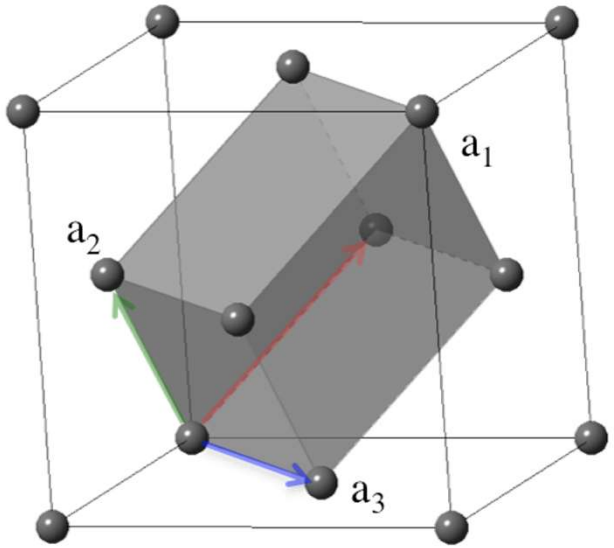
Reticoli di Bravais 3D



Cella di Wigner-Seitz





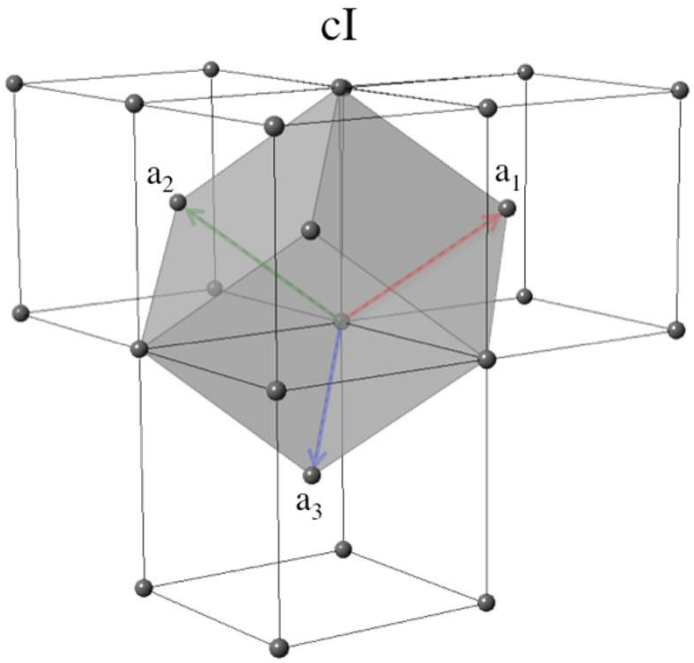


Reticolo FCC

Face centered cubic

ELEMENTS WITH THE MONATOMIC FACE-CENTERED CUBIC CRYSTAL STRUCTURE

ELEMENT	a (Å)	ELEMENT	a (Å)	ELEMENT	a (Å)
Ar	5.26 (4.2 K)	Ir	3.84	Pt	3.92
Ag	4.09	Kr	5.72 (58 K)	δ-Pu	4.64
Al	4.05	La	5.30	Rh	3.80
Au	4.08	Ne	4.43 (4.2 K)	Sc	4.54
Ca	5.58	Ni	3.52	Sr	6.08
Ce	5.16	Pb	4.95	Th	5.08
β-Co	3.55	Pd	3.89	Xe (58 K)	6.20
Cu	3.61	Pr	5.16	Yb	5.49



Reticolo BCC

↓

Body

ELEMENTS WITH THE MONATOMIC BODY-CENTERED CUBIC CRYSTAL STRUCTURE

ELEMENT	a (Å)	ELEMENT	a (Å)	ELEMENT	a (Å)
Ba	5.02	Li	3.49 (78 K)	Ta	3.31
Cr	2.88	Mo	3.15	Tl	3.88
Cs	6.05 (78 K)	Na	4.23 (5 K)	V	3.02
Fe	2.87	Nb	3.30	W	3.16
K	5.23 (5 K)	Rb	5.59 (5 K)		

Reticolo Diamante

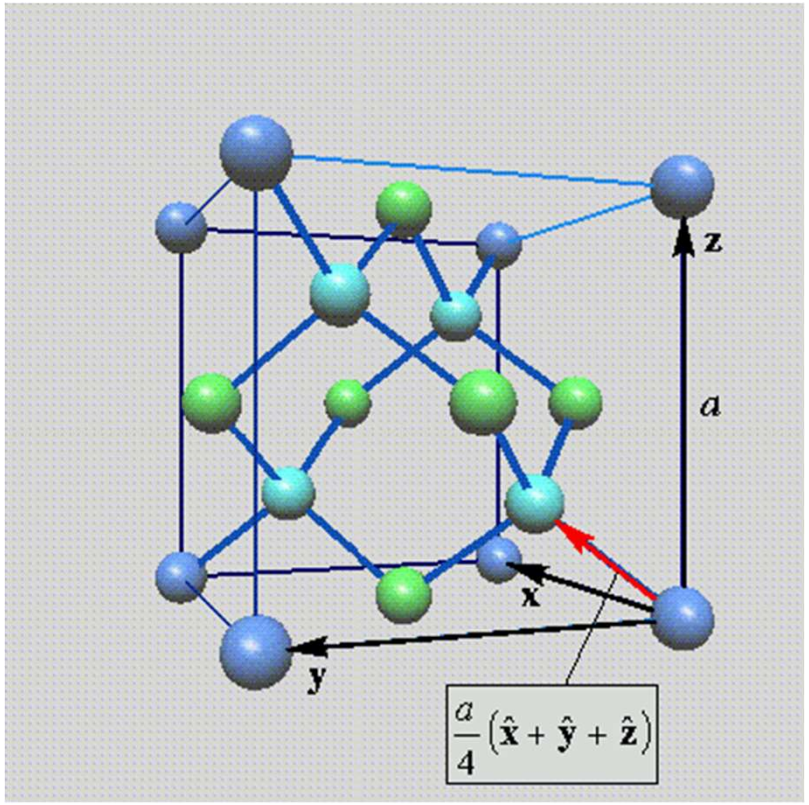
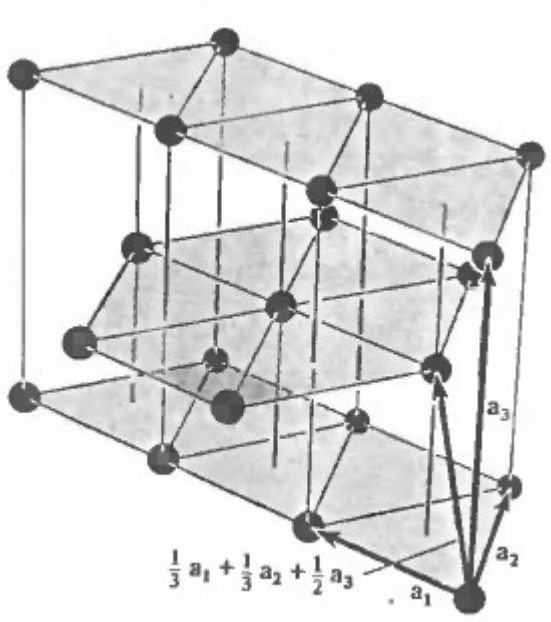


Table 4.3
ELEMENTS WITH THE DIAMOND CRYSTAL STRUCTURE

ELEMENT	CUBE SIDE a (Å)
C (diamond)	3.57
Si	5.43
Ge	5.66
α-Sn (grey)	6.49

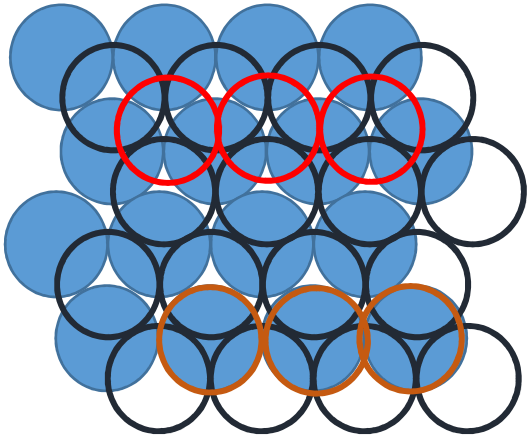


Reticolo esagonale compatto (HCP)

ELEMENTS WITH THE HEXAGONAL CLOSE-PACKED CRYSTAL STRUCTURE

ELEMENT	a (Å)	c	c/a	ELEMENT	a (Å)	c	c/a
Be	2.29	3.58	1.56	Os	2.74	4.32	1.58
Cd	2.98	5.62	1.89	Pr	3.67	5.92	1.61
Ce	3.65	5.96	1.63	Re	2.76	4.46	1.62
α-Co	2.51	4.07	1.62	Ru	2.70	4.28	1.59
Dy	3.59	5.65	1.57	Sc	3.31	5.27	1.59
Er	3.56	5.59	1.57	Tb	3.60	5.69	1.58
Gd	3.64	5.78	1.59	Ti	2.95	4.69	1.59
He (2 K)	3.57	5.83	1.63	Tl	3.46	5.53	1.60
Hf	3.20	5.06	1.58	Tm	3.54	5.55	1.57
Ho	3.58	5.62	1.57	Y	3.65	5.73	1.57
La	3.75	6.07	1.62	Zn	2.66	4.95	1.86
Lu	3.50	5.55	1.59	Zr	3.23	5.15	1.59
Mg	3.21	5.21	1.62		—	—	
Nd	3.66	5.90	1.61	"Ideal"			1.63

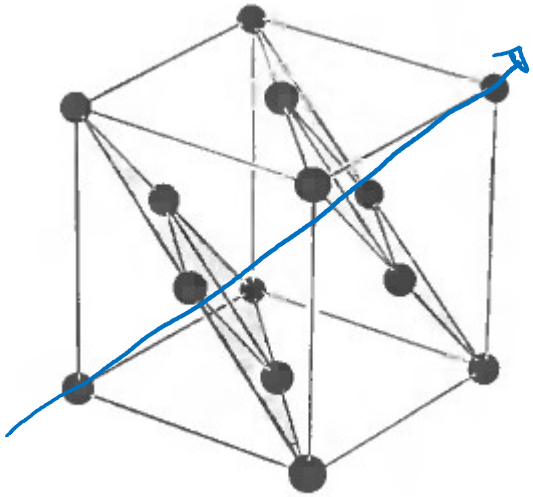
Reticoli Close-Packed



stocking ABC

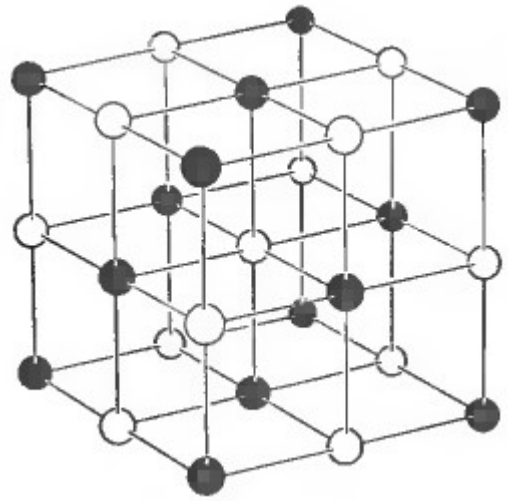
stocking

ABAB



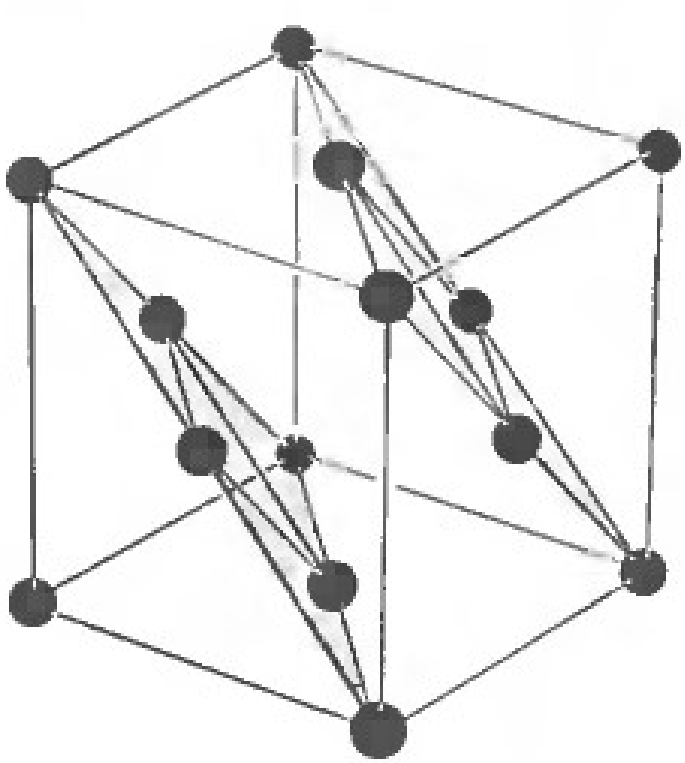
Packing : 74% (BCC: 68% SC: 52%)

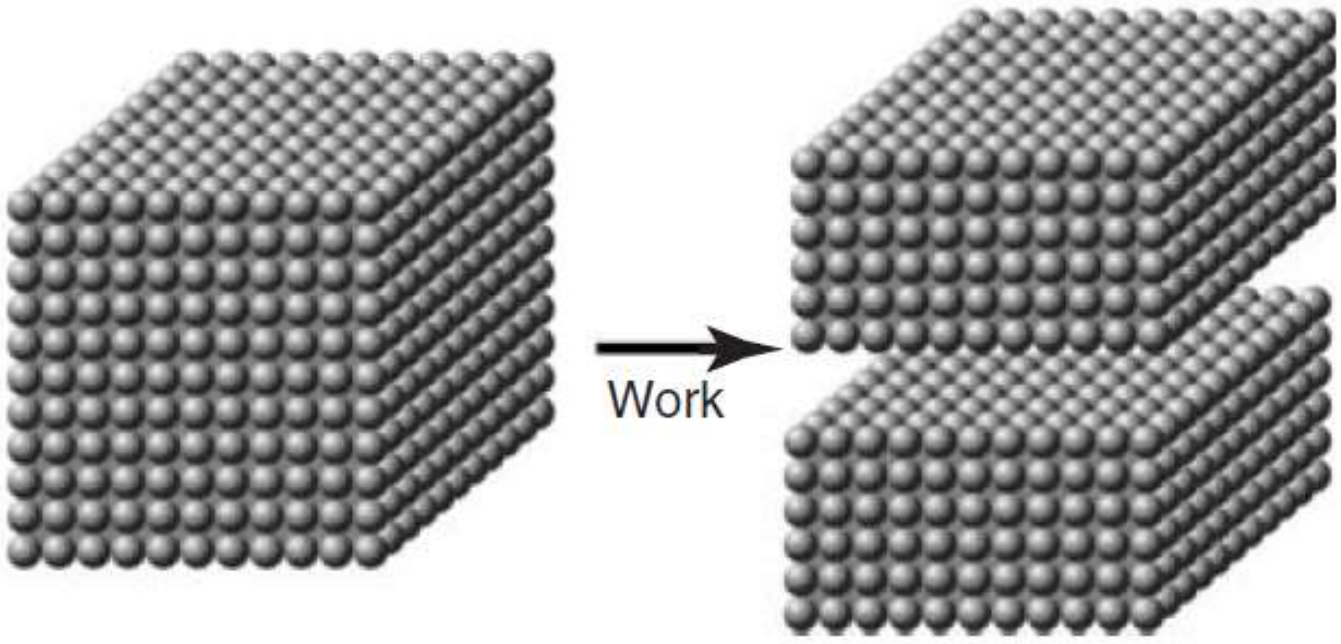
Introdurre una base è necessario per descrivere la struttura cristallina di composti. Ad esempio, il cloruro di sodio, ha una struttura in cui atomi di Na e di Cl si alternano in una struttura Simple Cubic.
La posso descrivere come una FCC con base



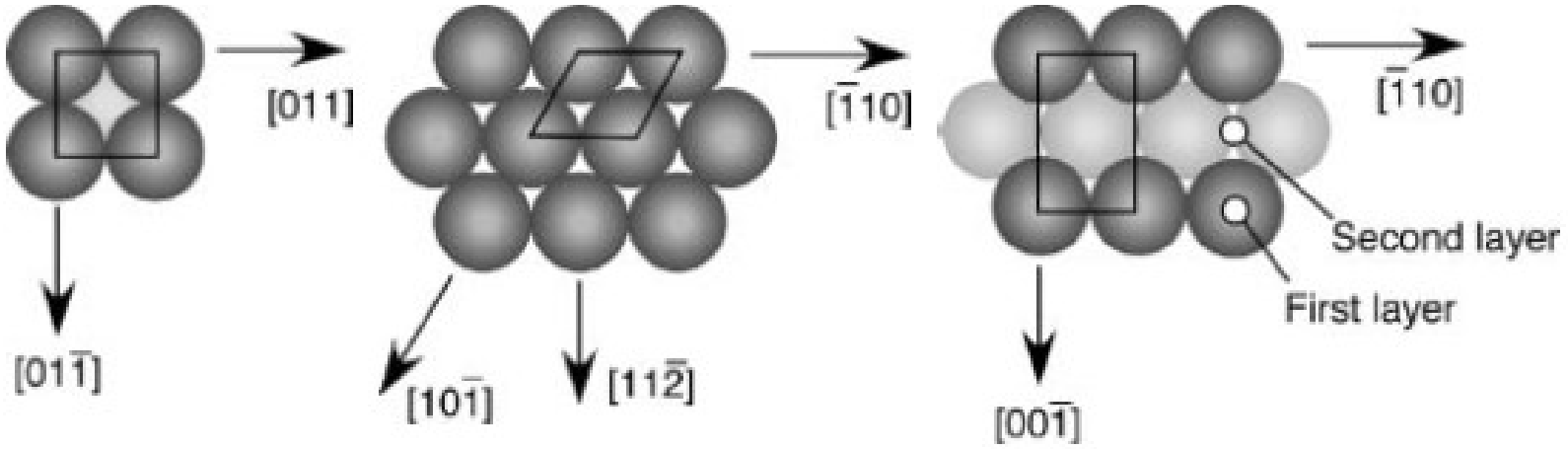
SOME COMPOUNDS WITH THE SODIUM CHLORIDE STRUCTURE

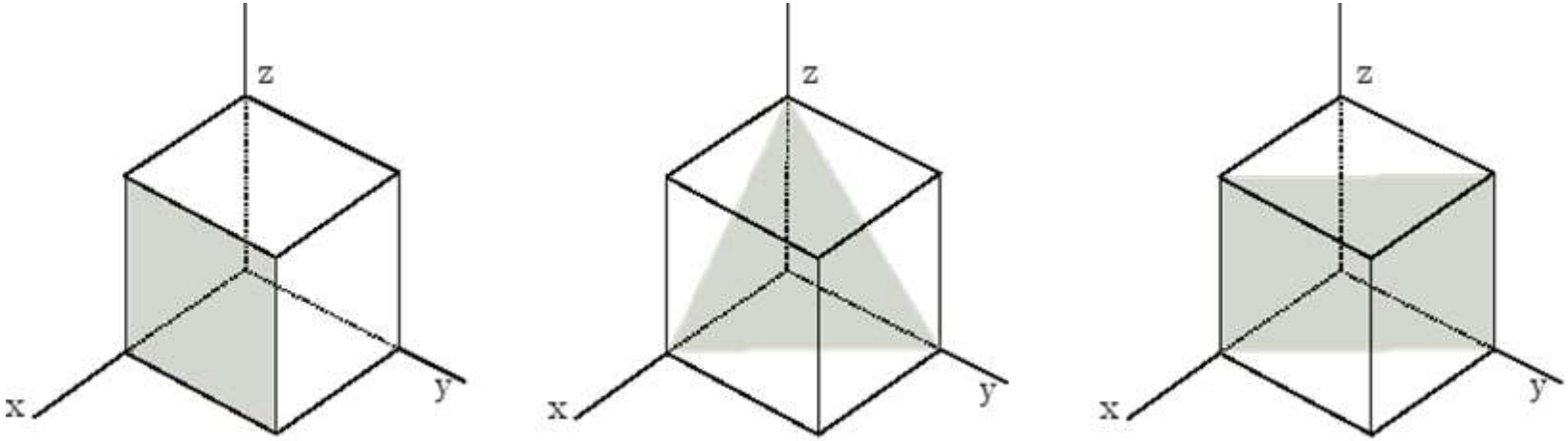
CRYSTAL	a (Å)	CRYSTAL	a (Å)	CRYSTAL	a (Å)
LiF	4.02	RbF	5.64	CaS	5.69
LiCl	5.13	RbCl	6.58	CaSe	5.91
LiBr	5.50	RbBr	6.85	CaTe	6.34
LiI	6.00	RbI	7.34	SrO	5.16
NaF	4.62	CsF	6.01	SrS	6.02
NaCl	5.64	AgF	4.92	SrSe	6.23
NaBr	5.97	AgCl	5.55	SrTe	6.47
NaI	6.47	AgBr	5.77	BaO	5.52
KF	5.35	MgO	4.21	BaS	6.39
KCl	6.29	MgS	5.20	BaSe	6.60
KBr	6.60	MgSe	5.45	BaTe	6.99
KI	7.07	CaO	4.81		



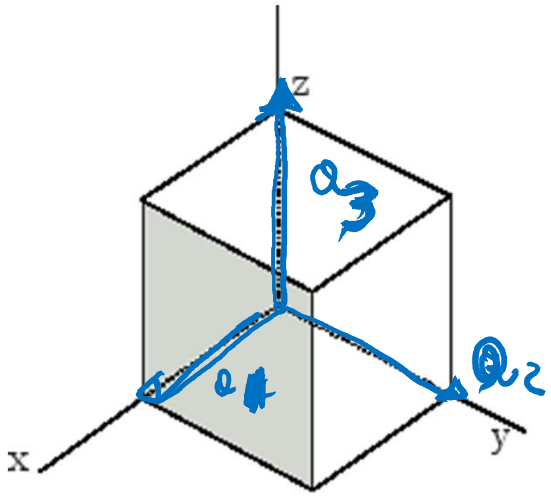

Work
Crystal
Creation of surface

Tre diverse superfici FCC

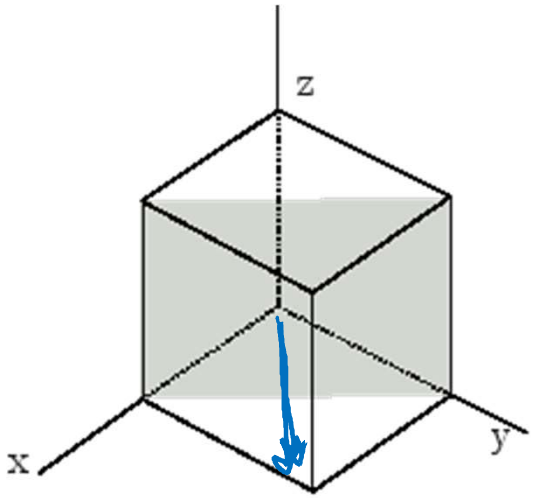




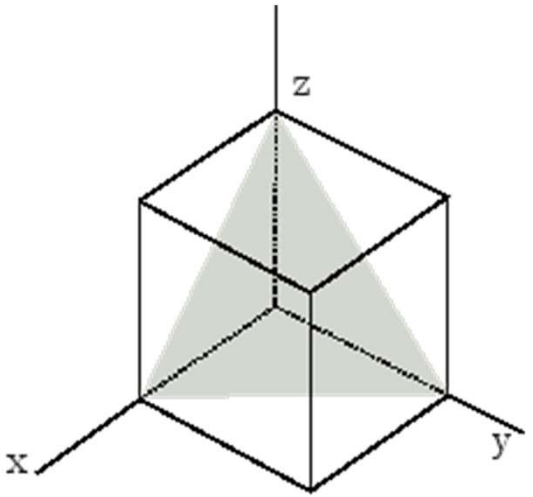
Indici di Miller



(100)



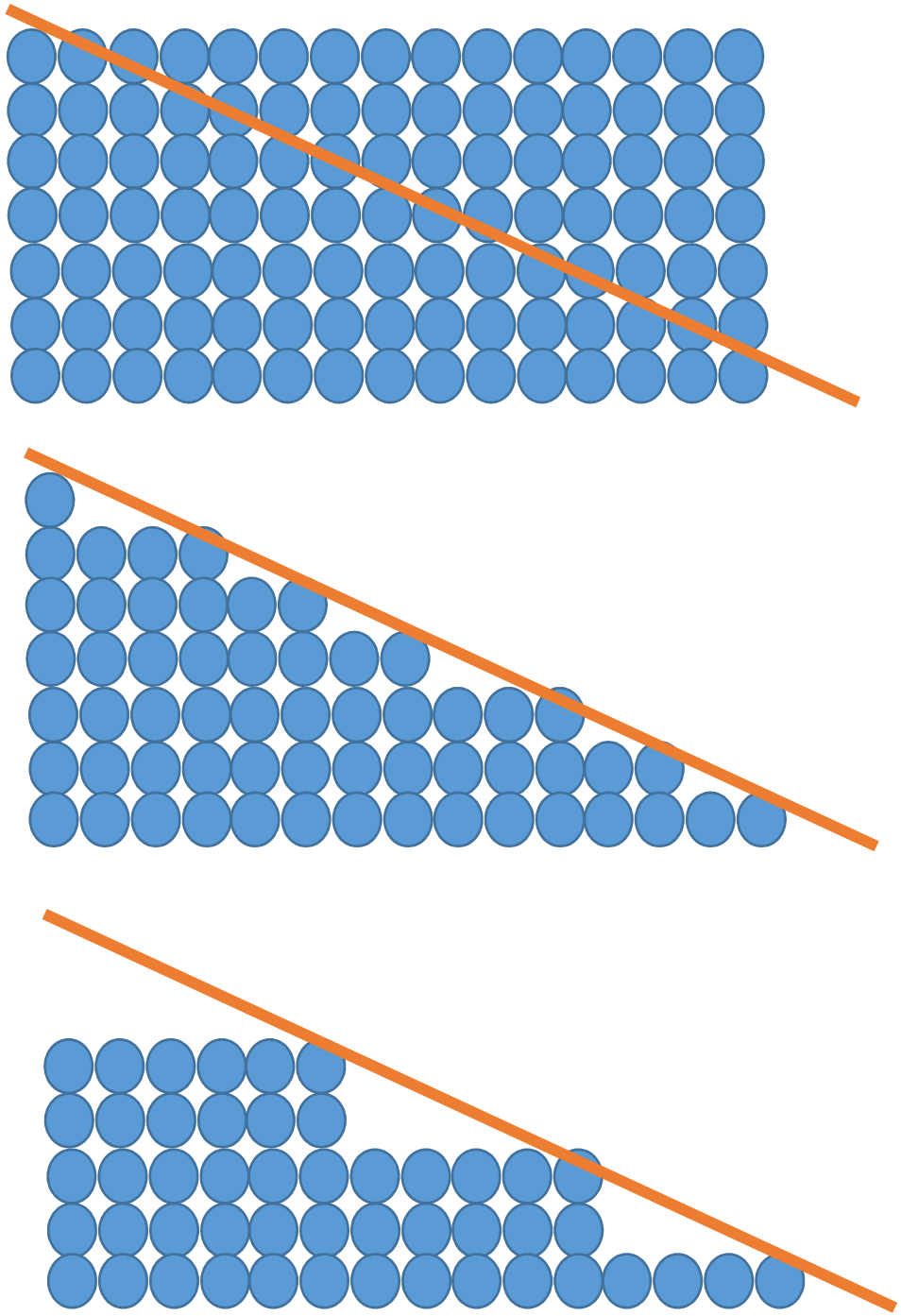
(110)



(111)

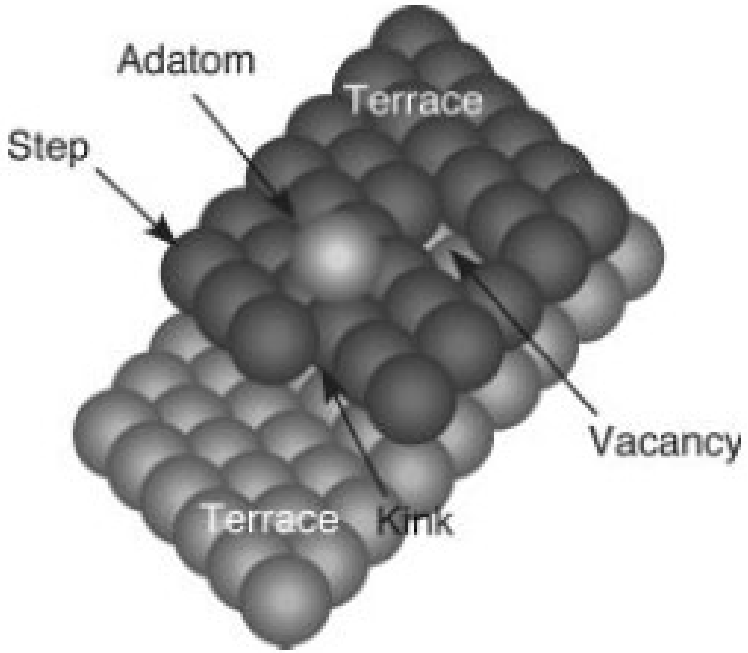
Il piano interseca i vettori della base in:

$(1, \infty, \infty)$ → prendo l'inverso → $(1, 0, 0)$ → indici di MILLER



FACETING

Superfici ad alti indici di MILLER hanno eccesso di energia che "ribesciano" creando terrazze più estese.


Adatom
Terrace
Step
Vacancy
Terrace
Kink