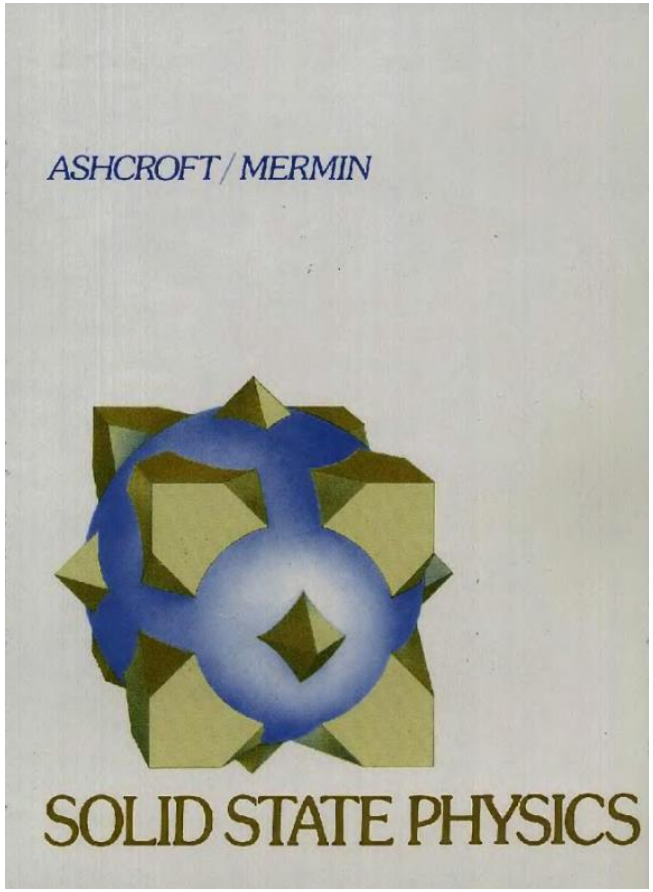
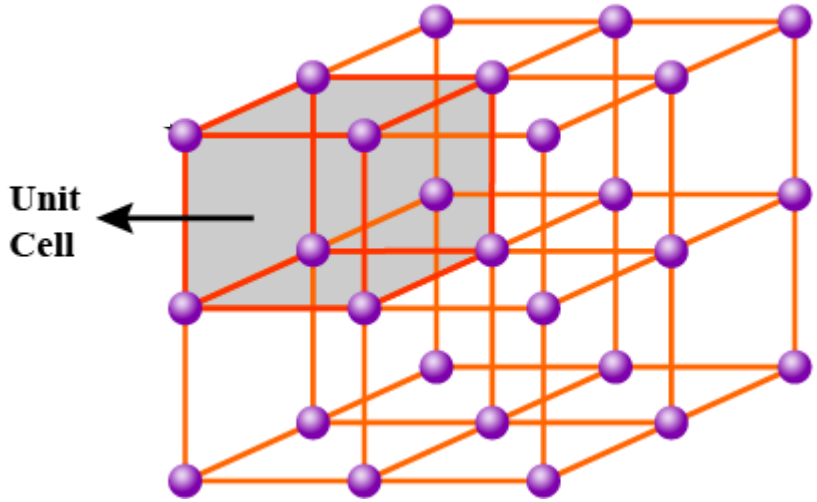


Capitoli 4 e 5

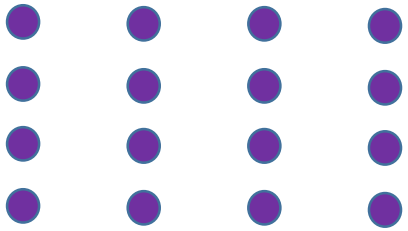
Il reticolo cristallino

è una distribuzione ordinata e periodica di punti che indicano la posizione che atomi, molecole o gruppi di atomi o molecole hanno nella loro disposizione. La cella unitaria è un volume (superficie nel caso 2D) che, se ripetuto nelle 3 (2) direzioni mi riproduce reticolo



3D

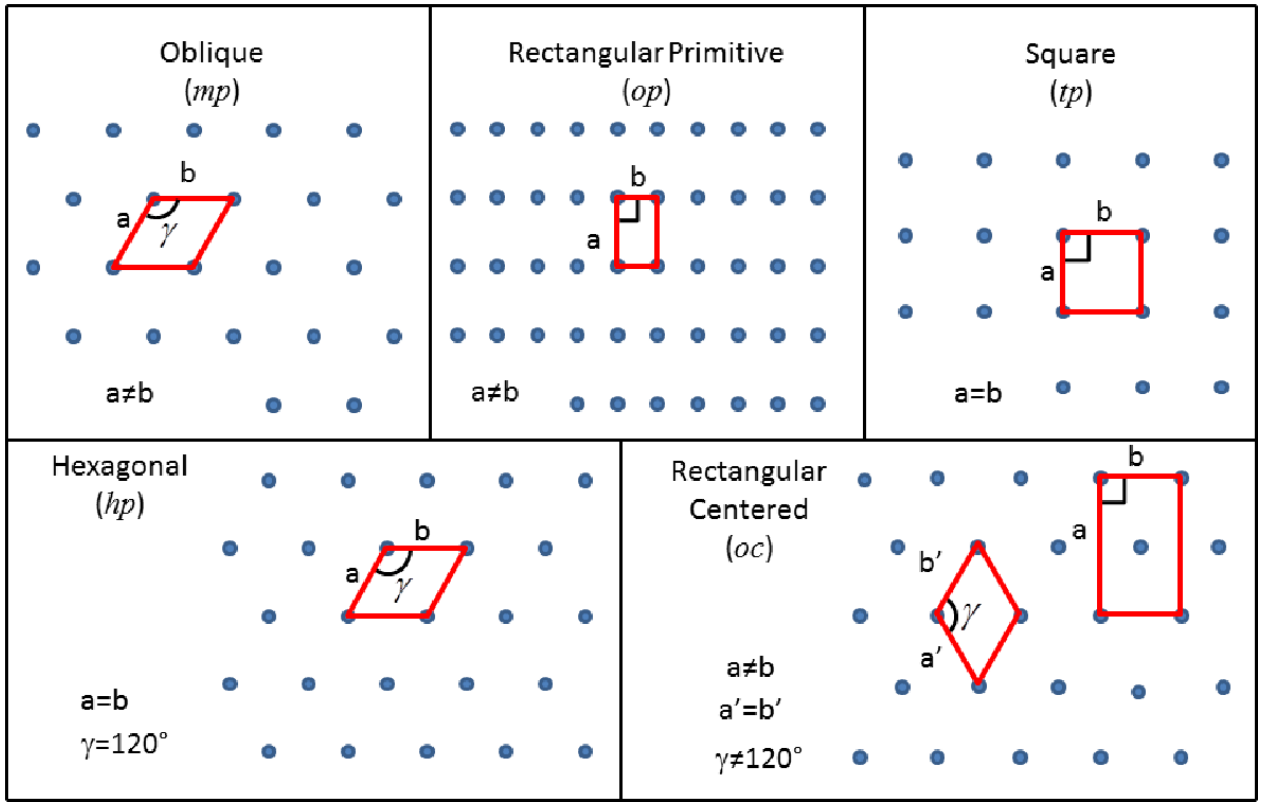
Nel caso 2D la cella sarà ovviamente 2D…



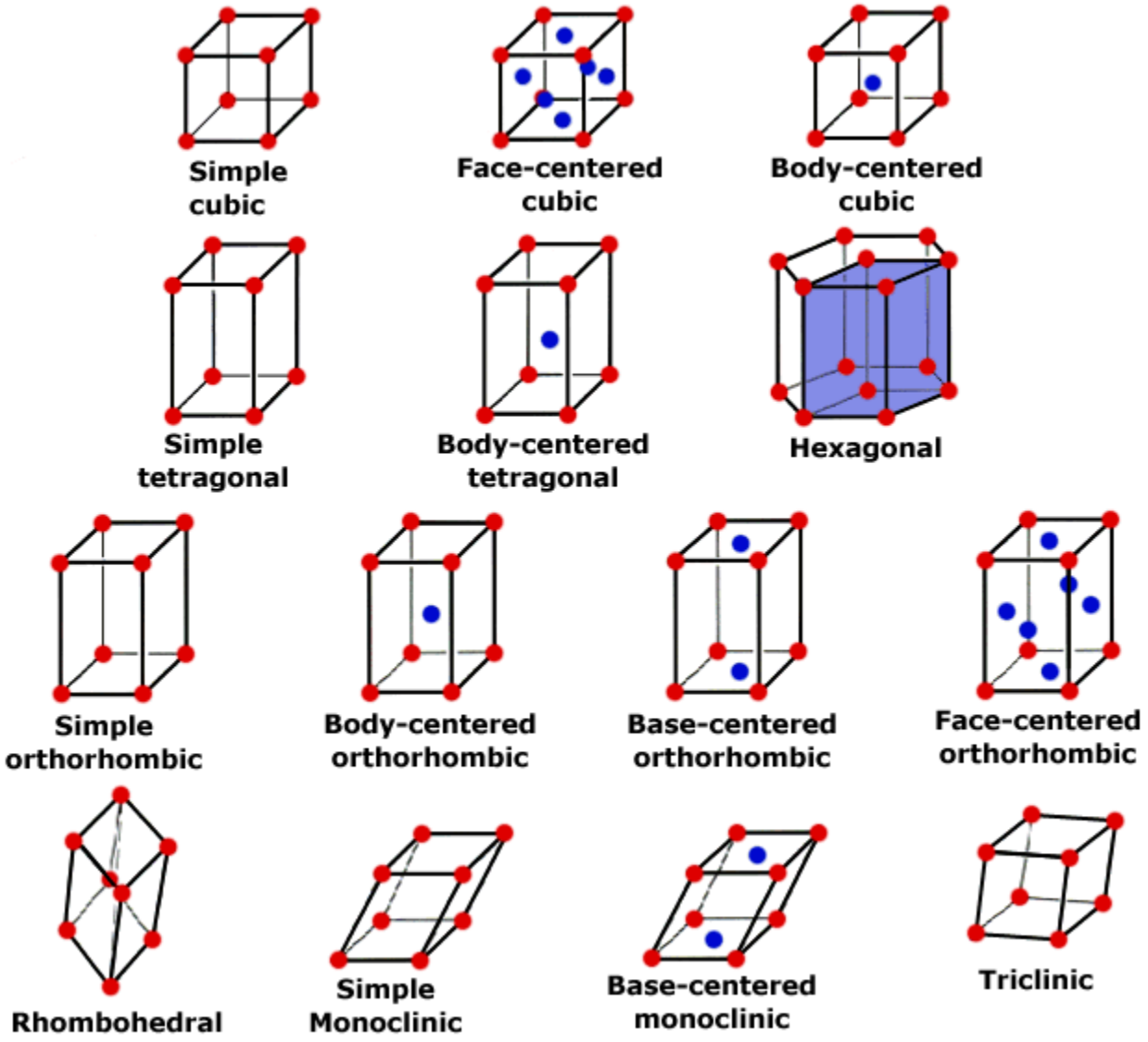
2D

L’insieme di reticoli possibili con cui si può ricoprire una superficie o un volume è noto come insieme di Reticoli di Bravais. Ho 5 possibilità in 2D e 14 in 3D.

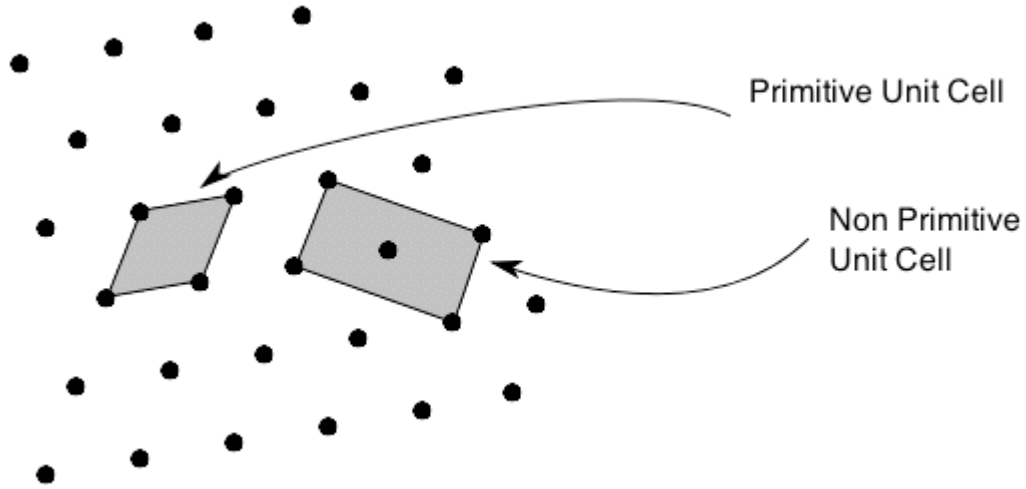
Reticoli di Bravais 2D

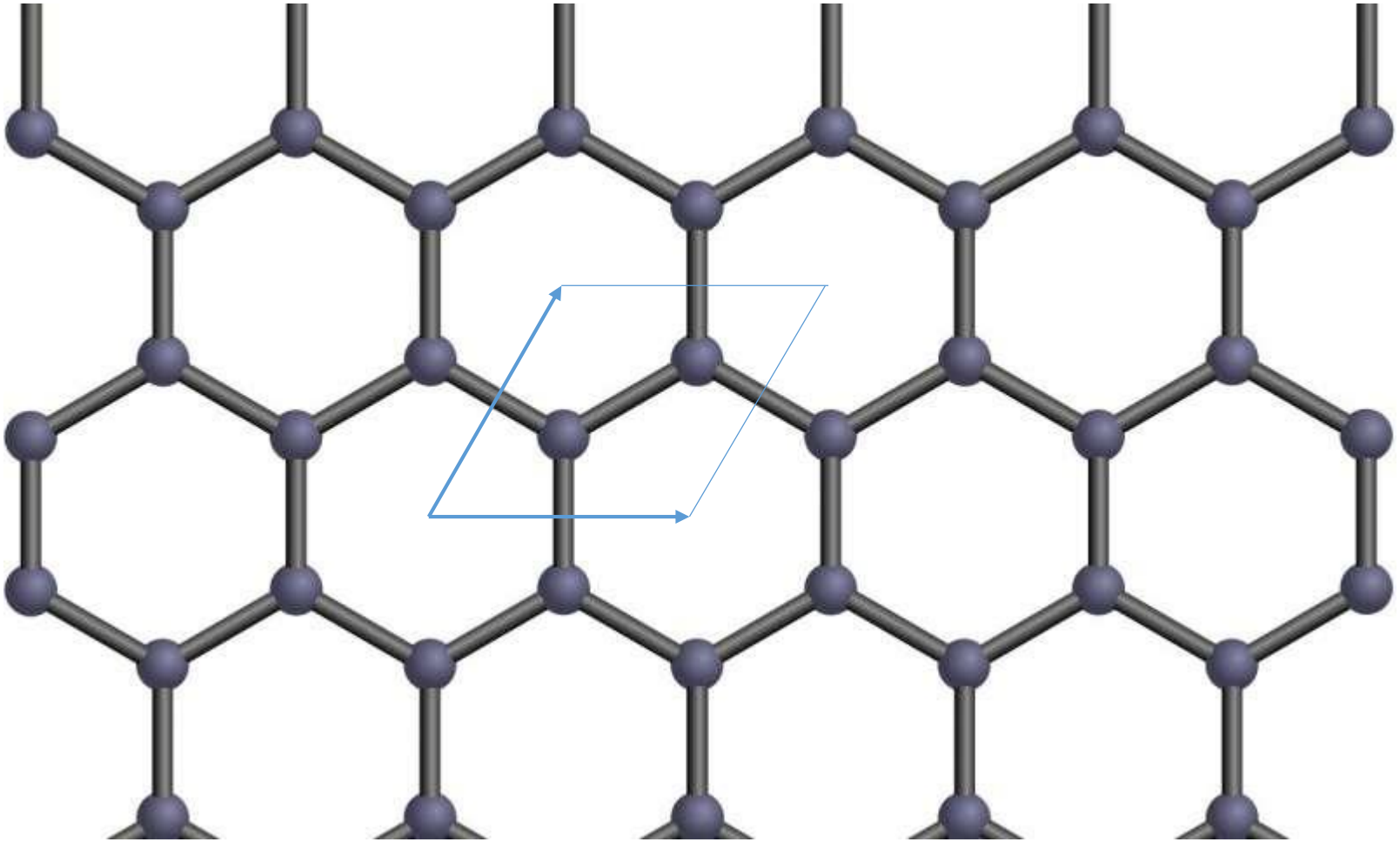


Reticoli di Bravais 3D



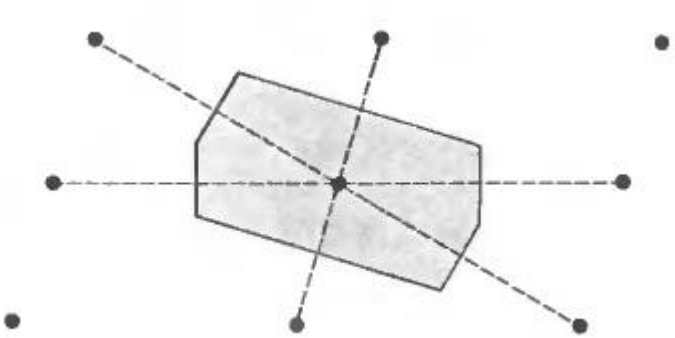
La scelta delle celle non è univoca. La cella di minimo volume o area è detta cella primitiva. Essa copre tutto lo spazio attraverso traslazioni pari ai vettori del reticolo di Bravais.
Celle unitarie non primitive (dette anche convenzionali) possono essere scelte perché più intuitive o più facili da utilizzare.

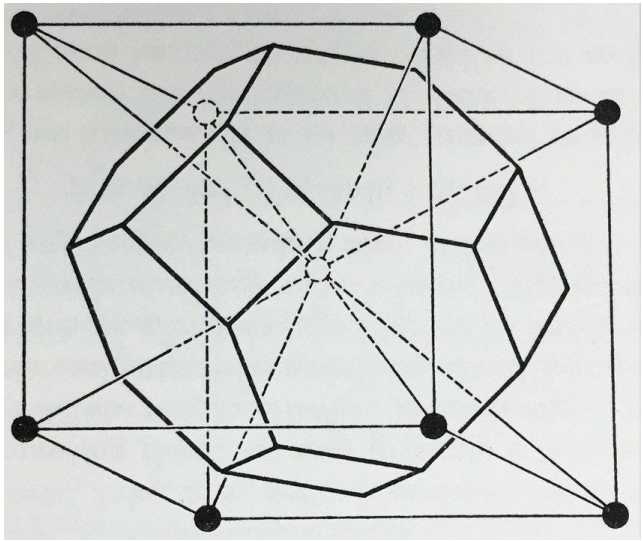


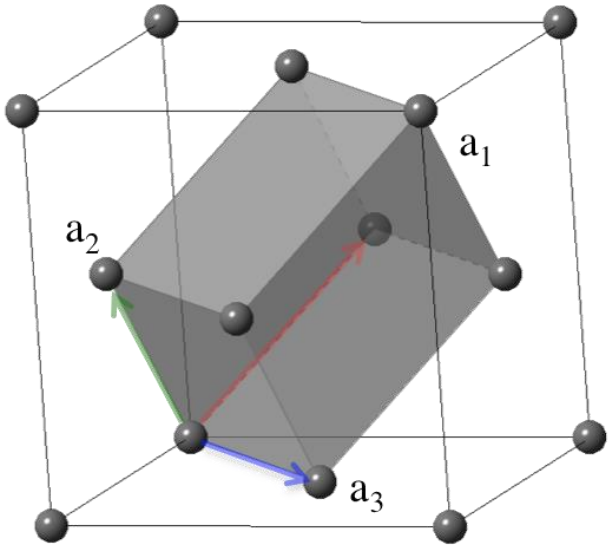


Cella di Wigner-Seitz

E’ la cella primitiva centrata rispetto ad un punto del reticolo e più simmetrica rispetto ad esso. Si trova con la procedura indicata a fianco,



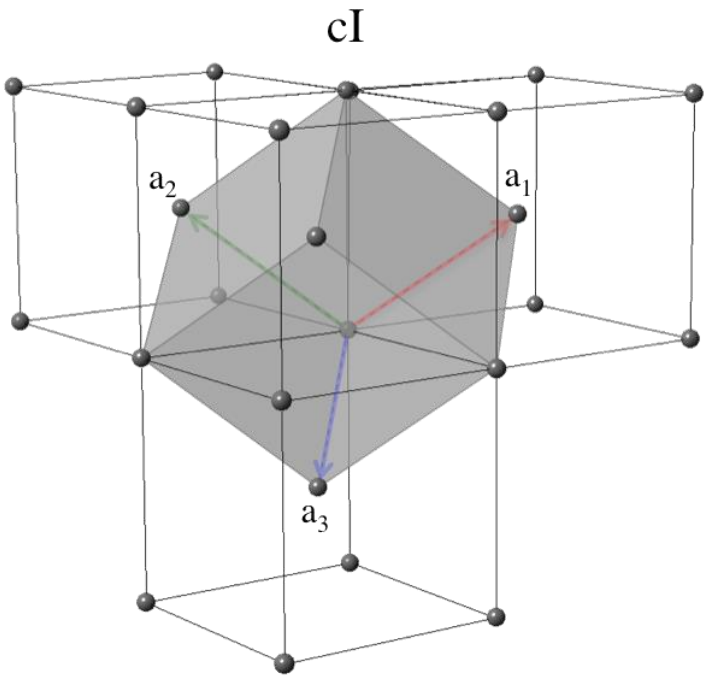




Reticolo FCC

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

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

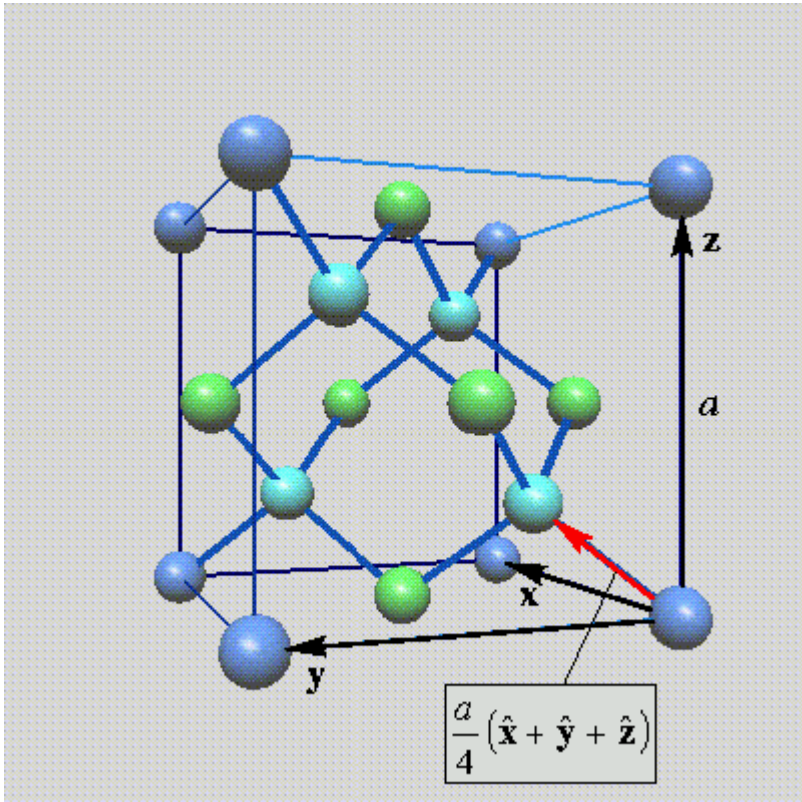
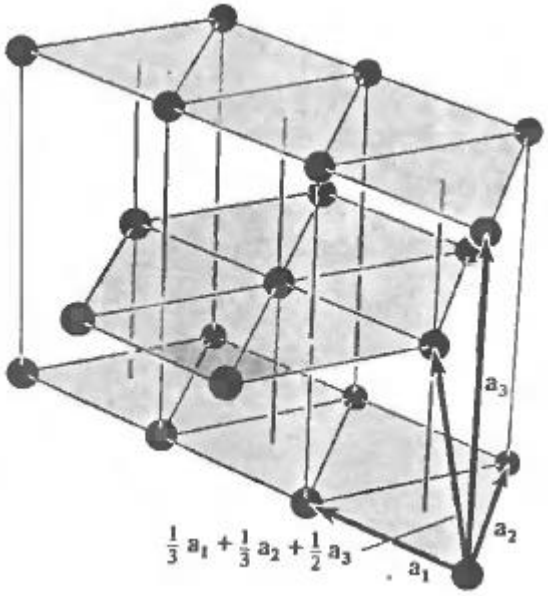


Table 4.3
ELEMENTS WITH THE DIAMOND CRYSTAL STRUCTURE

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

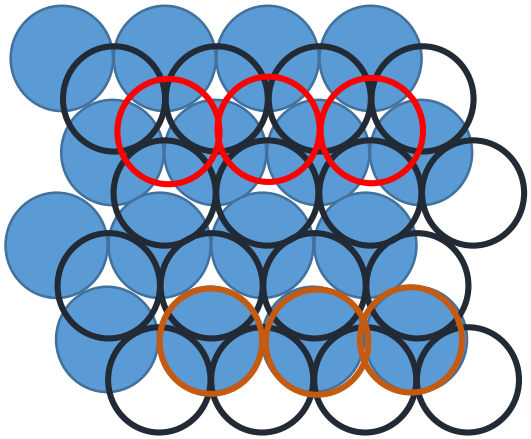


Reticolo esagonale compatto (HCP)

ELEMENTS WITH THE HEXAGONAL CLOSE-PACKED CRYSTAL STRUCTURE

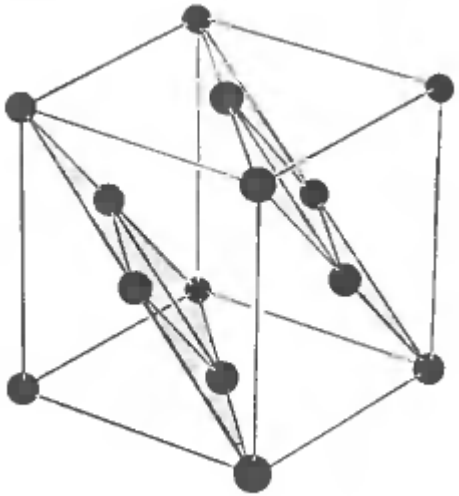
ELEMENT	a (Å)	c	c/a	ELEMENT	a (Å)	c	c/a
Be	2.29	3.58	1.56	Os	2.74	4.32	1.58
Cd	2.98	5.62	1.89	Pr	3.67	5.92	1.61
Ce	3.65	5.96	1.63	Re	2.76	4.46	1.62
α-Co	2.51	4.07	1.62	Ru	2.70	4.28	1.59
Dy	3.59	5.65	1.57	Sc	3.31	5.27	1.59
Er	3.56	5.59	1.57	Tb	3.60	5.69	1.58
Gd	3.64	5.78	1.59	Ti	2.95	4.69	1.59
He (2 K)	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



Stacking ABC

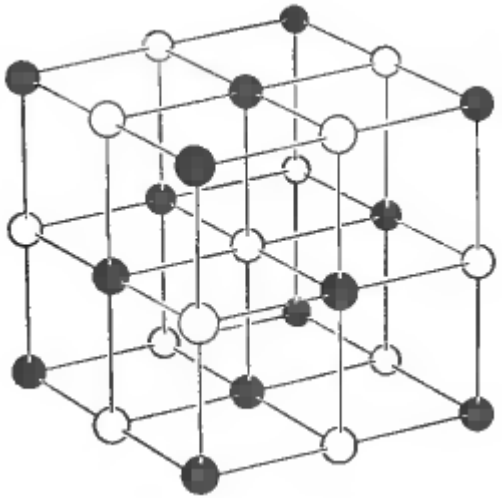
Stacking ABAB



Lo stacking ABC è il reticolo FCC.

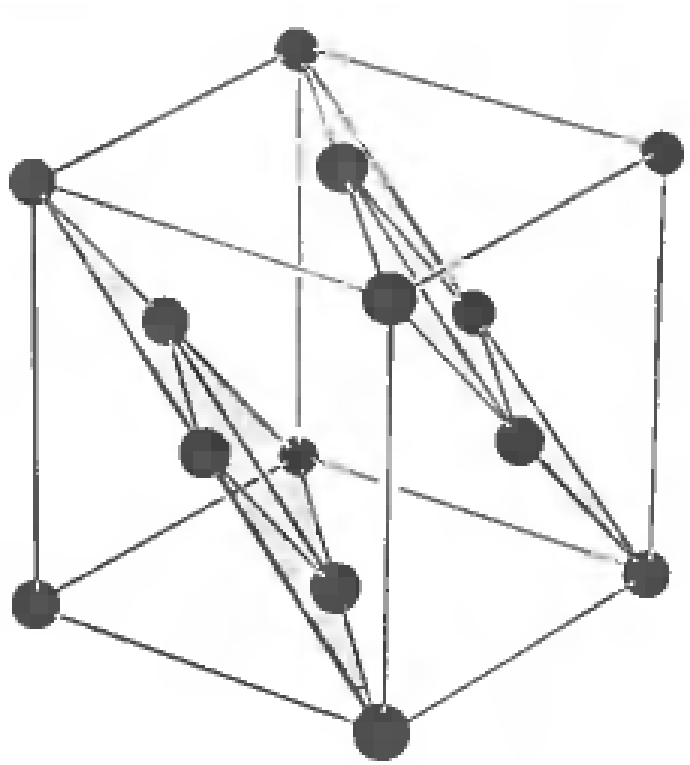
FCC e HCP permettono il massimo impacchettamento di sfere in un volume in termini di spazio occupato

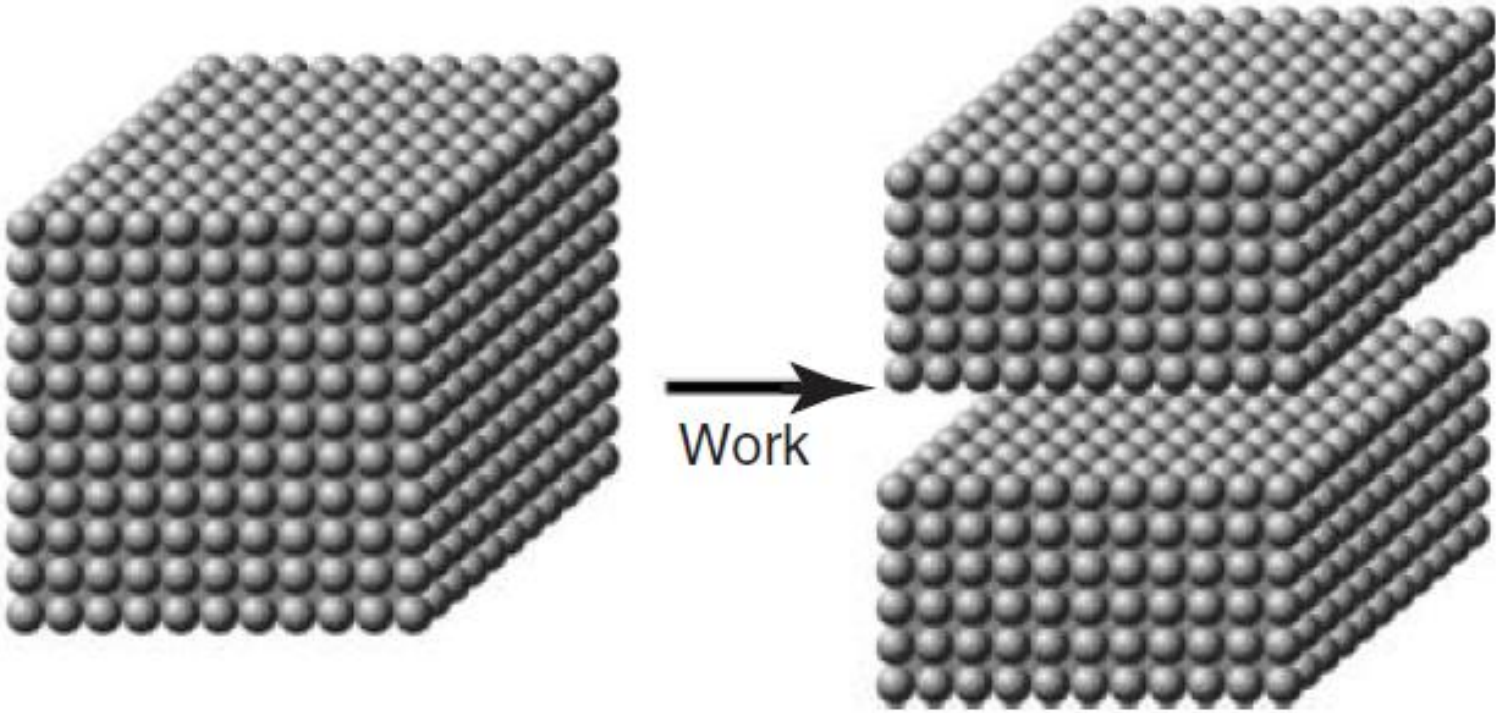
Packing : 74% (BCC: 68% SC: 52%)



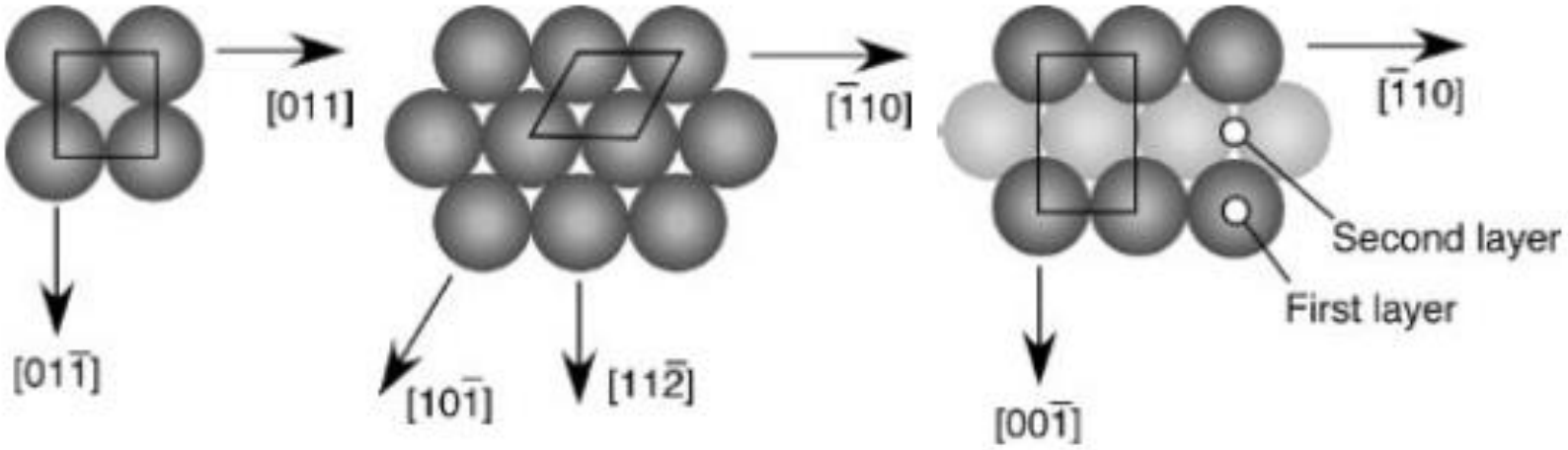
SOME COMPOUNDS WITH THE SODIUM CHLORIDE STRUCTURE

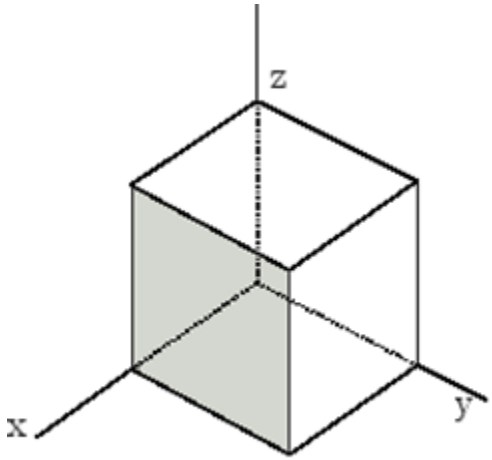
CRYSTAL	a (Å)	CRYSTAL	a (Å)	CRYSTAL	a (Å)
LiF	4.02	RbF	5.64	CaS	5.69
LiCl	5.13	RbCl	6.58	CaSe	5.91
LiBr	5.50	RbBr	6.85	CaTe	6.34
LiI	6.00	RbI	7.34	SrO	5.16
NaF	4.62	CsF	6.01	SrS	6.02
NaCl	5.64	AgF	4.92	SrSe	6.23
NaBr	5.97	AgCl	5.55	SrTe	6.47
NaI	6.47	AgBr	5.77	BaO	5.52
KF	5.35	MgO	4.21	BaS	6.39
KCl	6.29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



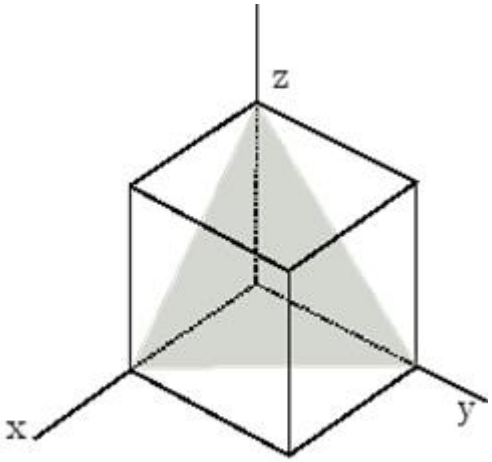

Work
Crystal
Creation of surface

Tre diverse superfici FCC

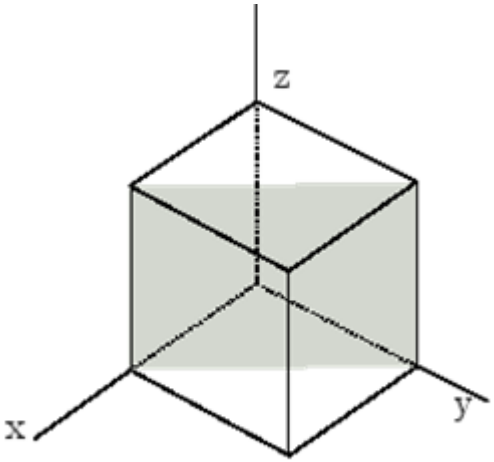




(100)

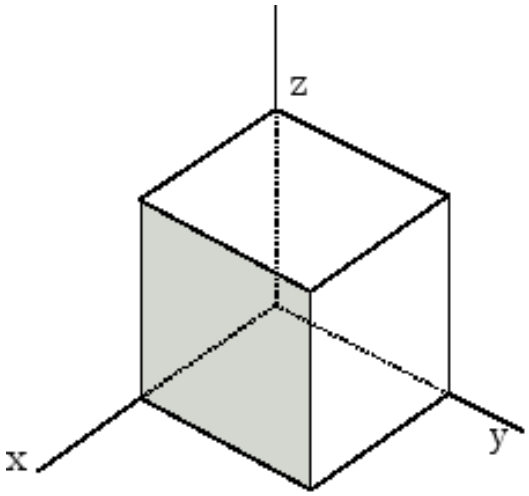


(111)



(110)

Indici di Miller



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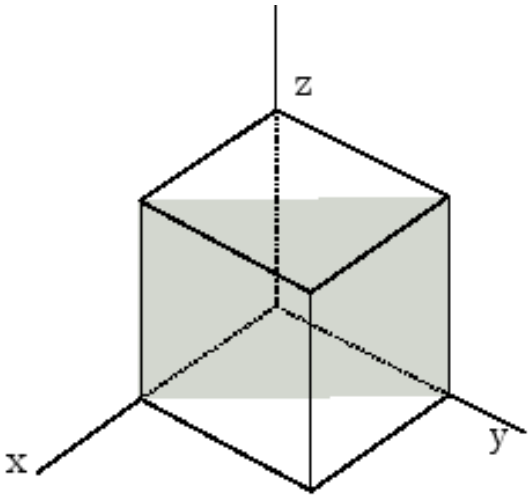

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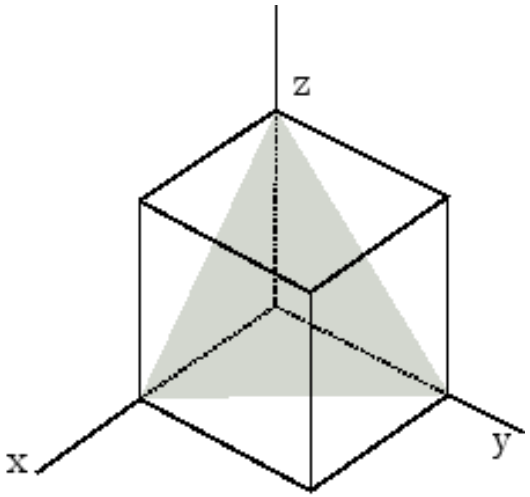
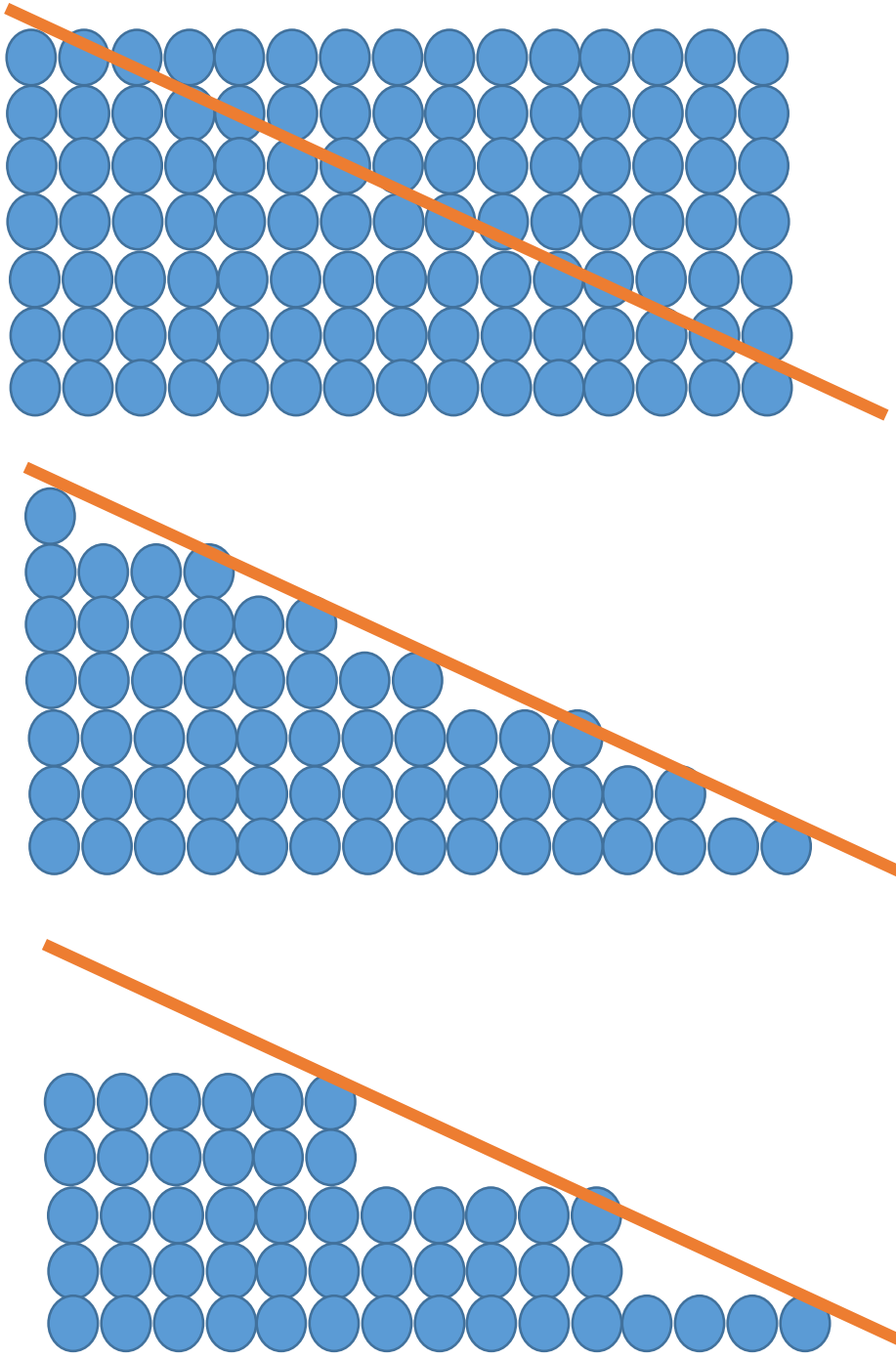
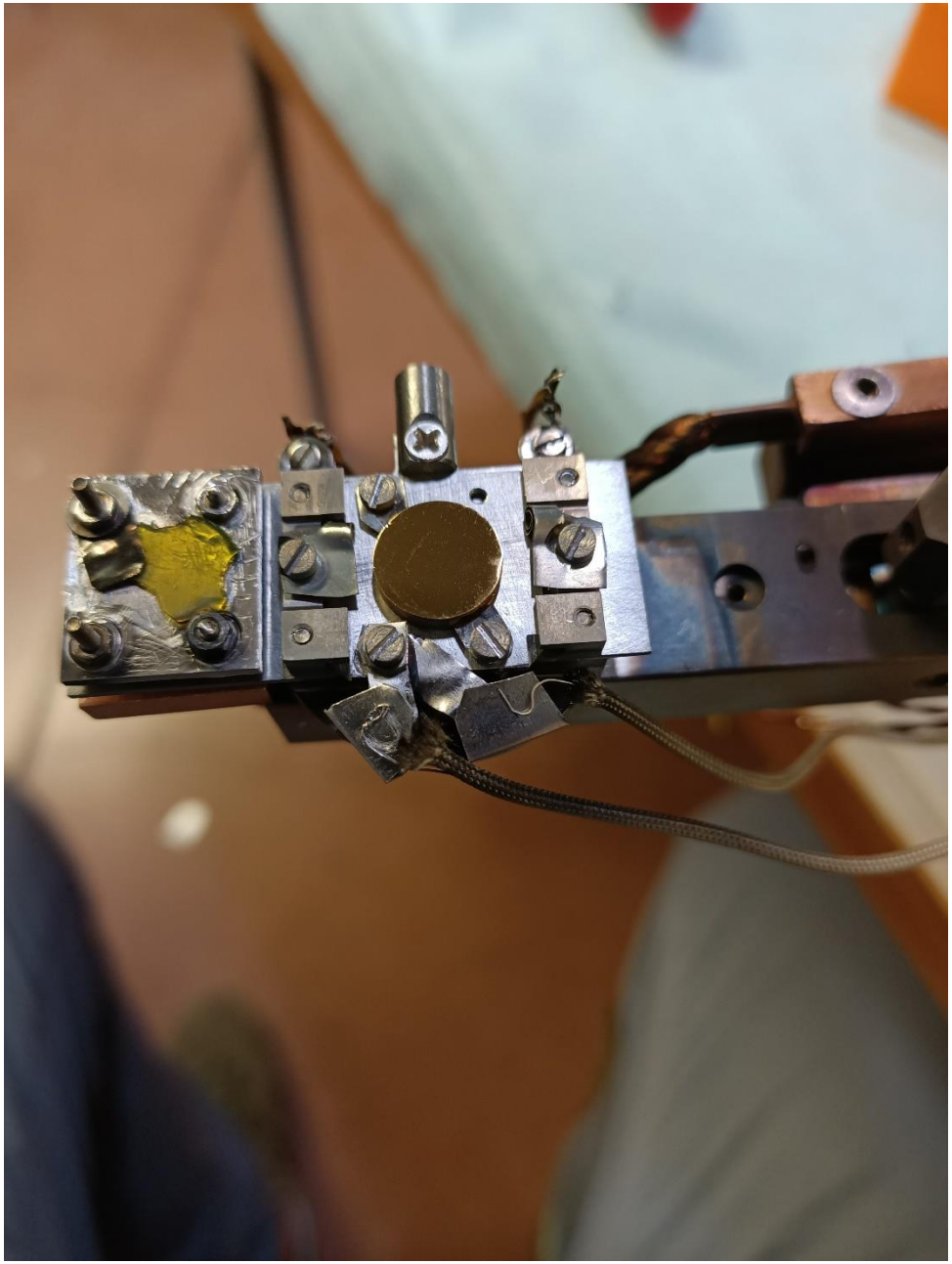


(111)

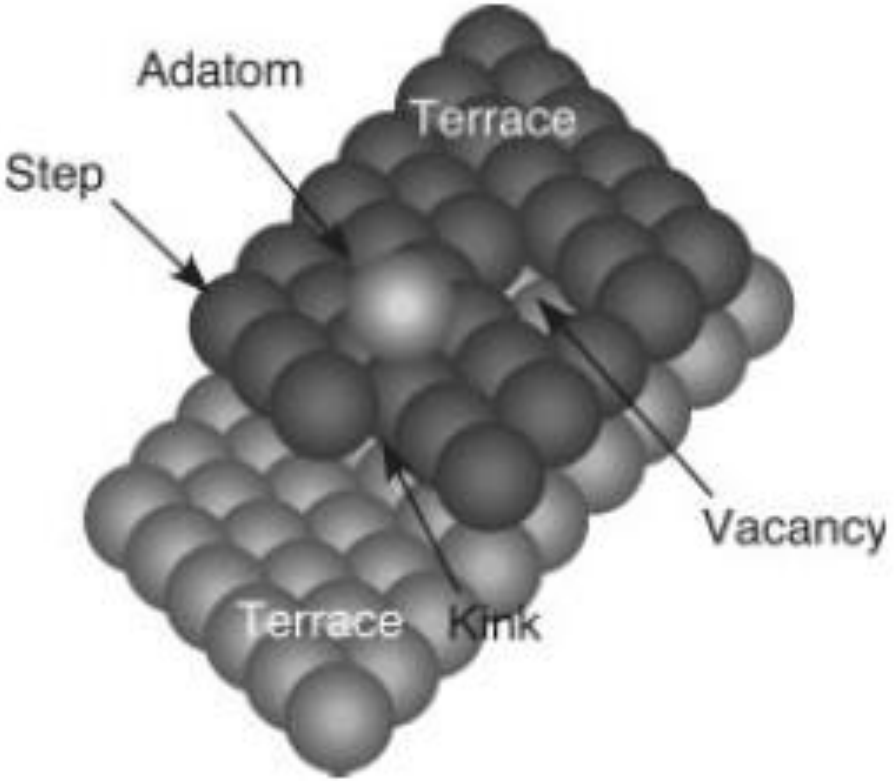


Faceting



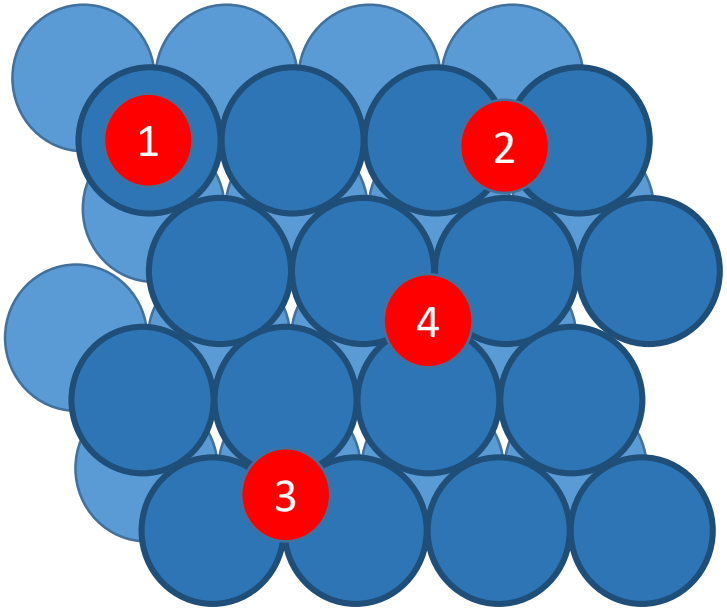
Campione di Au(111)
Single crystal

Montaggio su portacampioni
per misure di spettroscopia

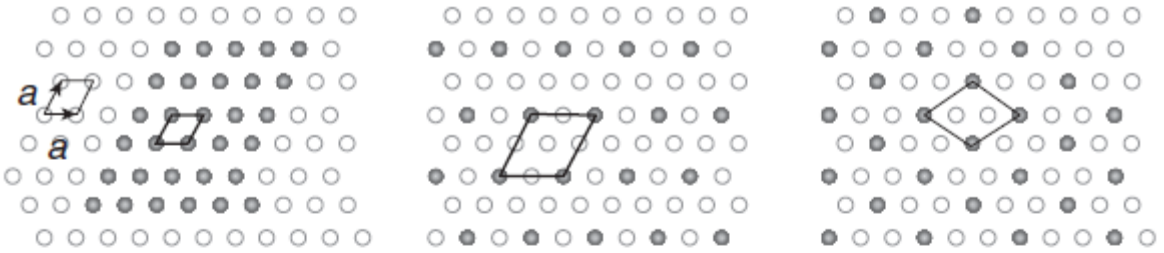


Siti di adsorbimento:

1. On Top
2. Bridge
3. Hollow HCP
4. Hollow FCC

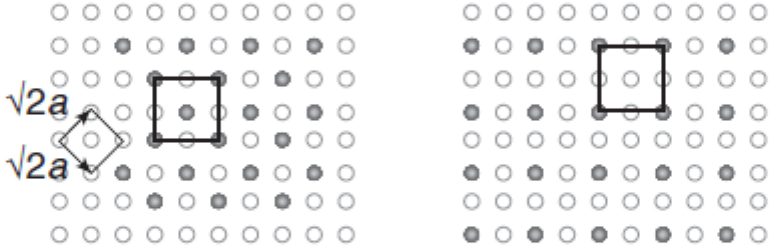


Esempi di strutture commensurate con il substrato



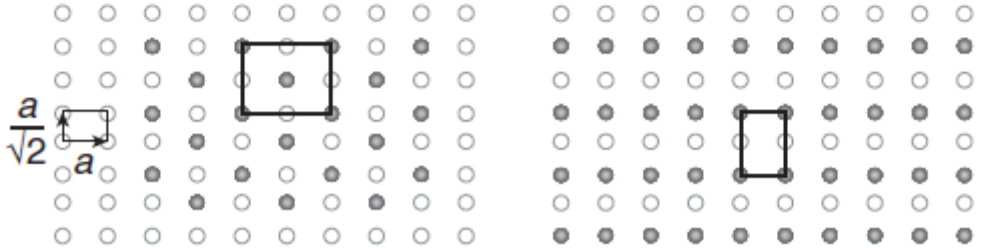
(i) (1×1) (ii) (2×2) (iii) $(\sqrt{3} \times \sqrt{3})$

(a)



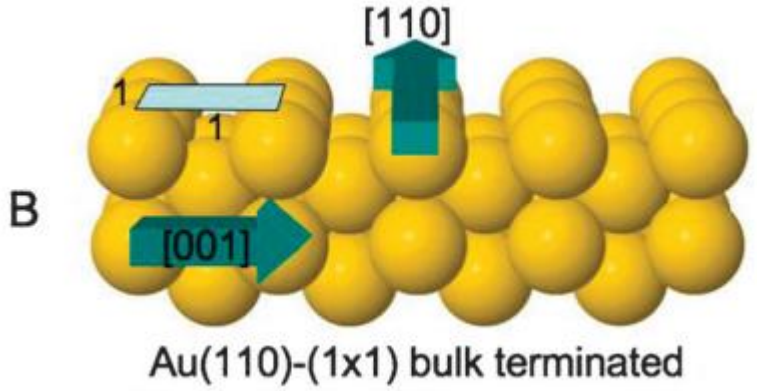
(i) $c(2 \times 2)=(\sqrt{2} \times \sqrt{2})R45°$ (ii) (2×2)

(b)

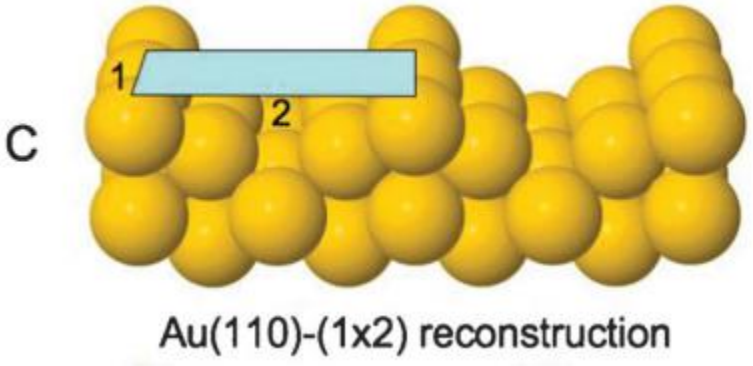


(i) $c(2 \times 2)$ (ii) (1×2)

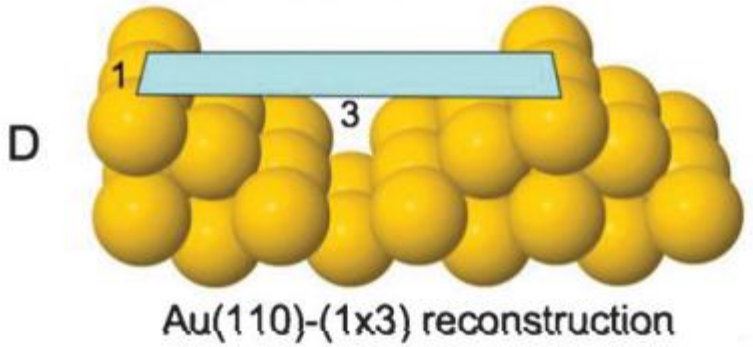
Superficie Au(110) terminata bulk (quella che mi aspetto semplicemente da un taglio del cristallo)



Superficie Au(110) che osservo sperimentalmente, dovuta al rilassamento. (minimizza l'energia)



Superficie Au(110) dopo un possible lifting della ricostruzione missing row, dovuto all'interazione con specie adsorbite



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