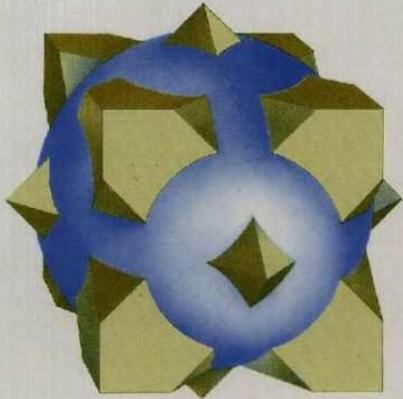


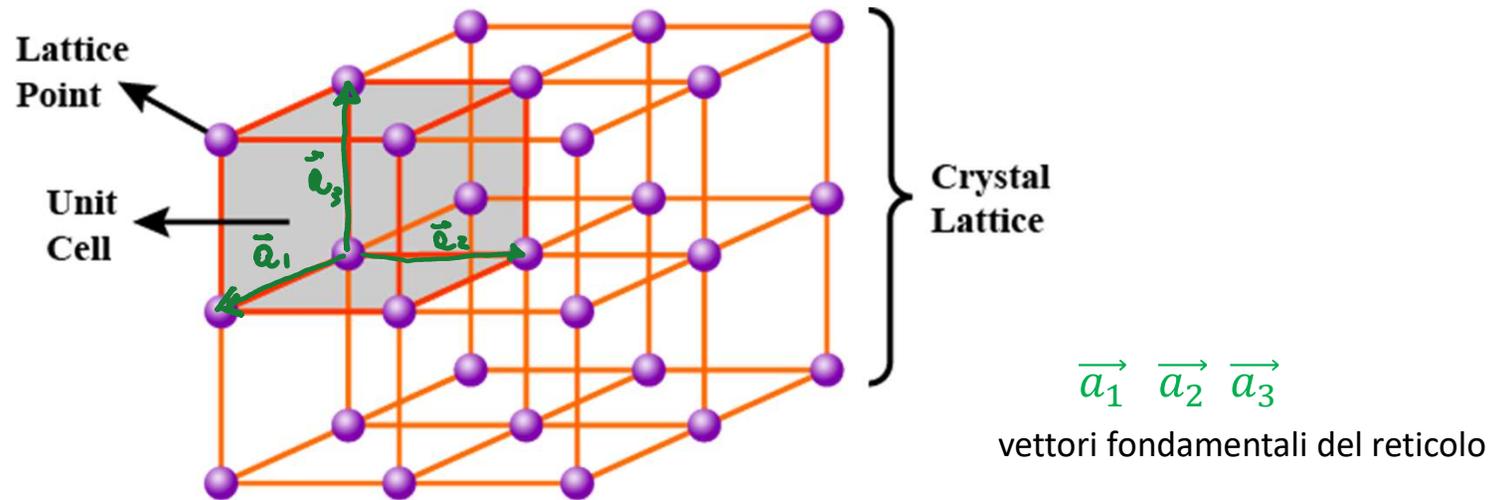
ASHCROFT/MERMIN



SOLID STATE PHYSICS

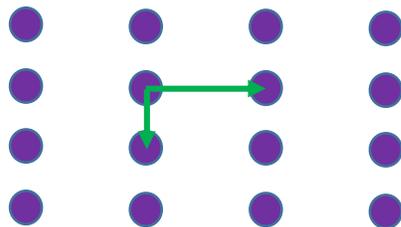
**Capitoli 4 e 5**

**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 si riproduce reticolo



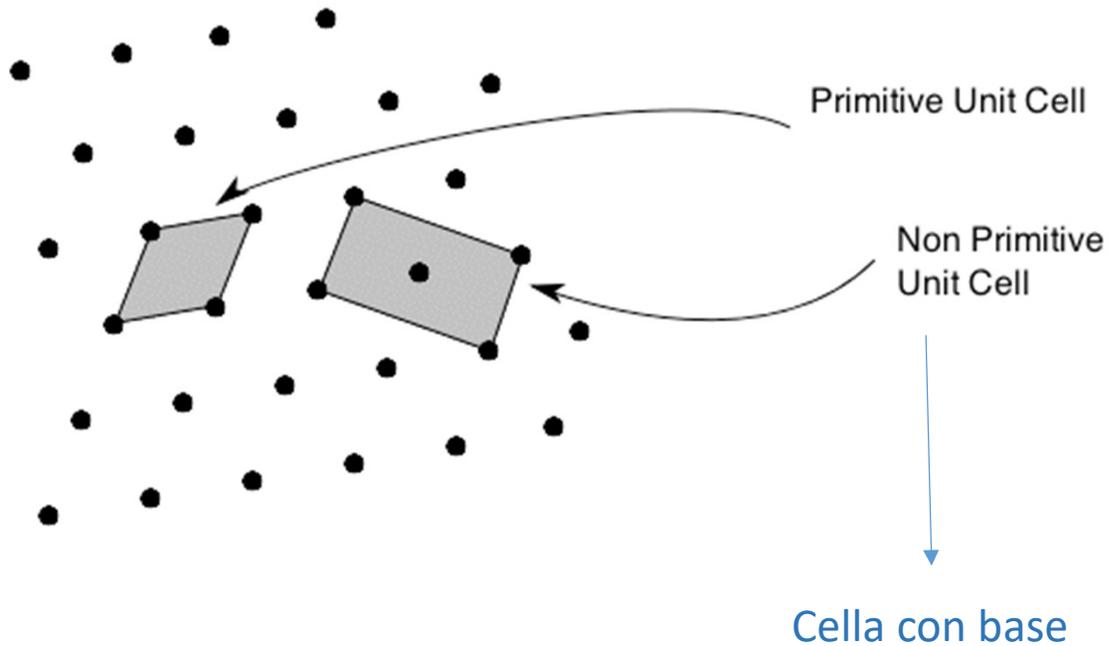
3D

Nel caso 2D la cella sarà ovviamente 2D...

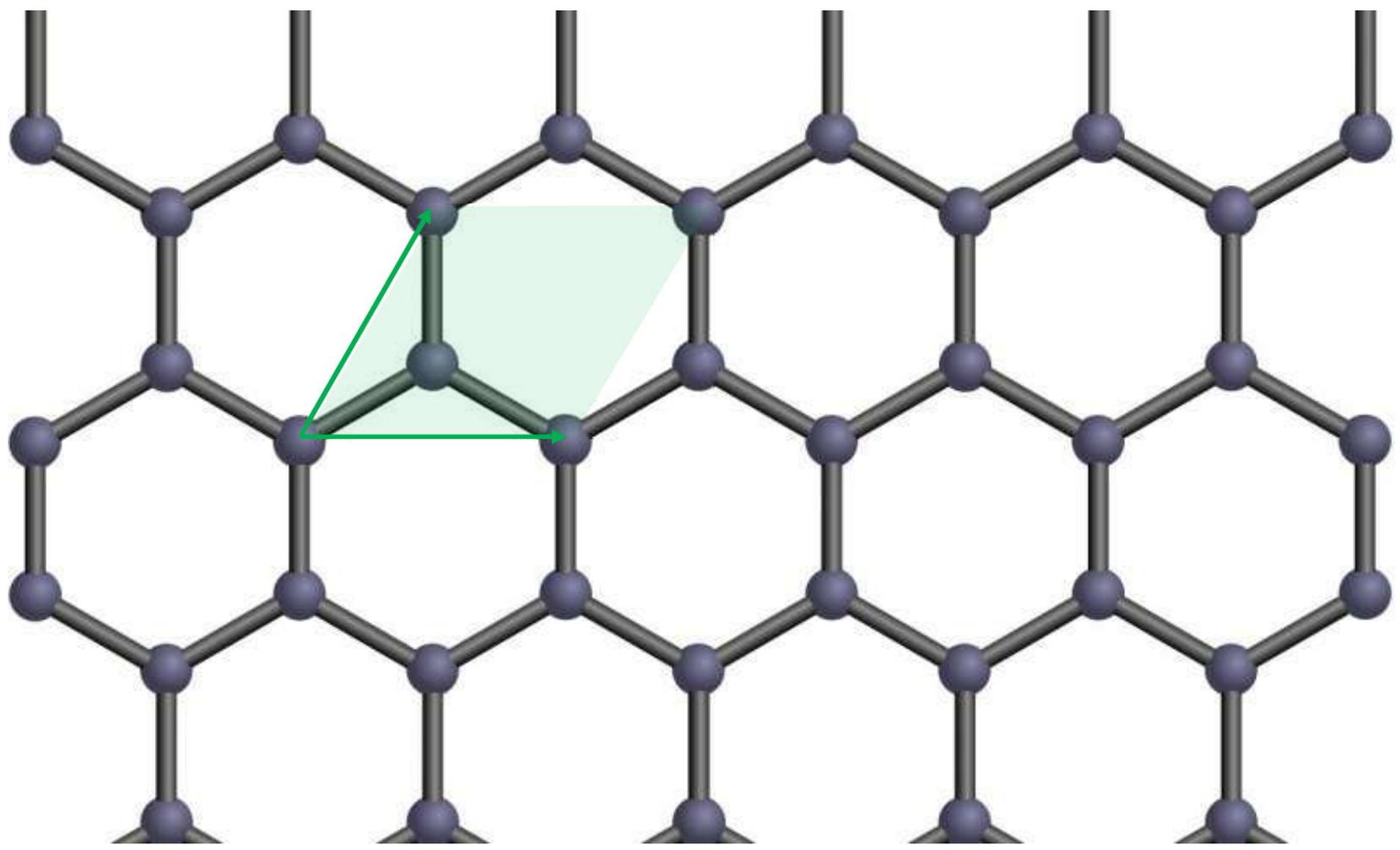


2D

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.

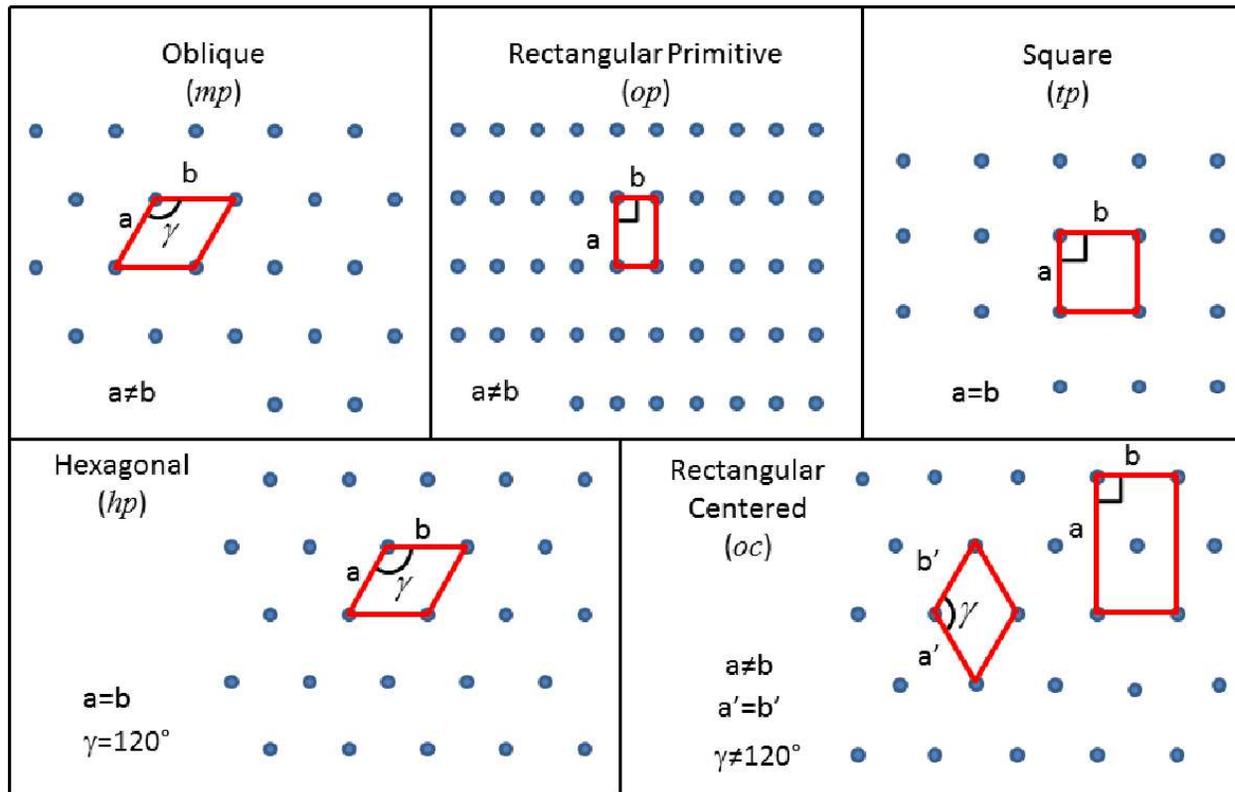


Esempio : il grafene ha reticolo esagonale con base



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.

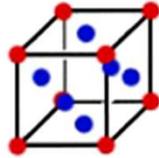
## Reticoli di Bravais 2D



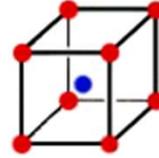
# Reticoli di Bravais 3D



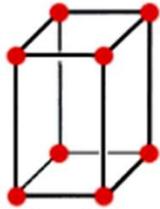
**Simple cubic**



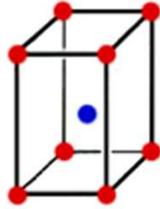
**Face-centered cubic**



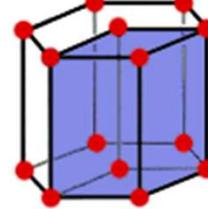
**Body-centered cubic**



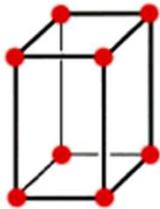
**Simple tetragonal**



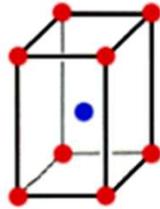
**Body-centered tetragonal**



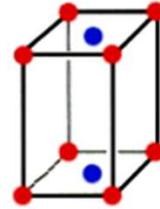
**Hexagonal**



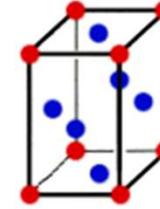
**Simple orthorhombic**



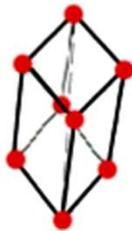
**Body-centered orthorhombic**



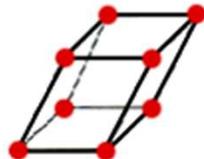
**Base-centered orthorhombic**



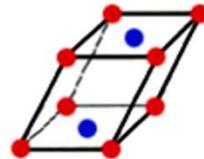
**Face-centered orthorhombic**



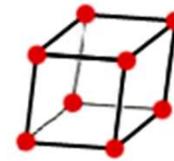
**Rhombohedral**



**Simple Monoclinic**



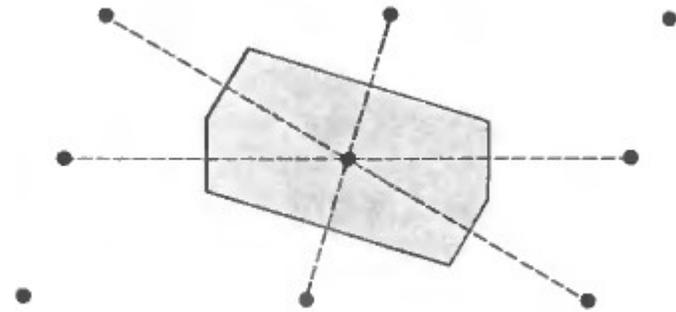
**Base-centered monoclinic**



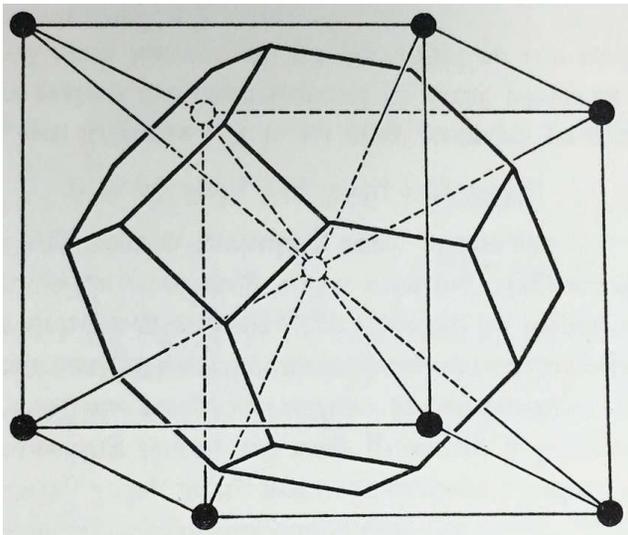
**Triclinic**

# 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:

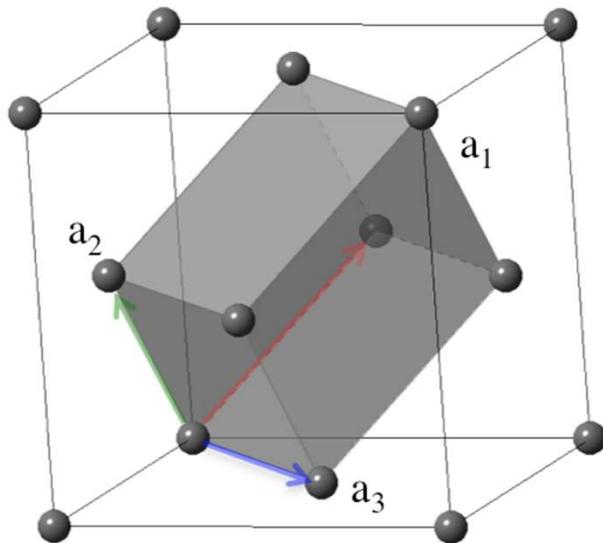


1. Collego un punto ai primi vicini
  2. Traccio le mediane
- La cella ottenuta è la cella di WS



BCC, cella di W-S

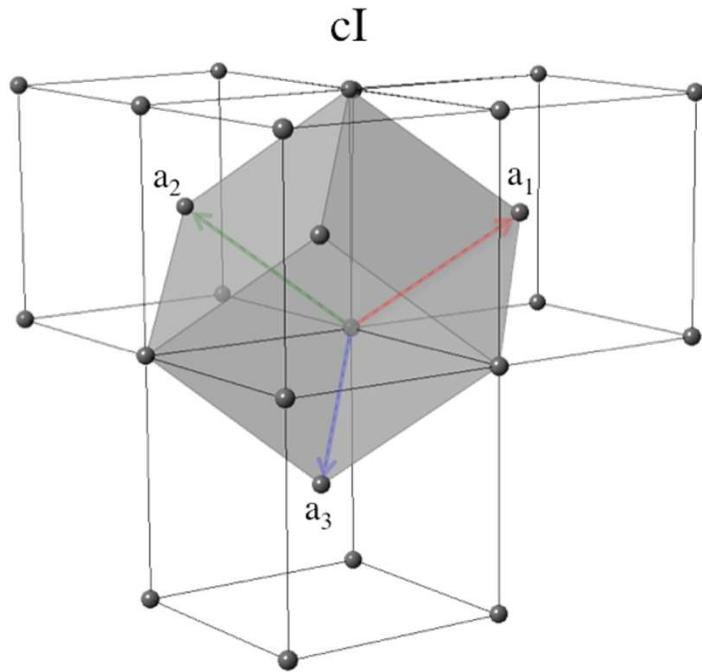
Nel caso 3D le mediane diventano dei piani...



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)	$\delta$ -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
$\beta$ -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

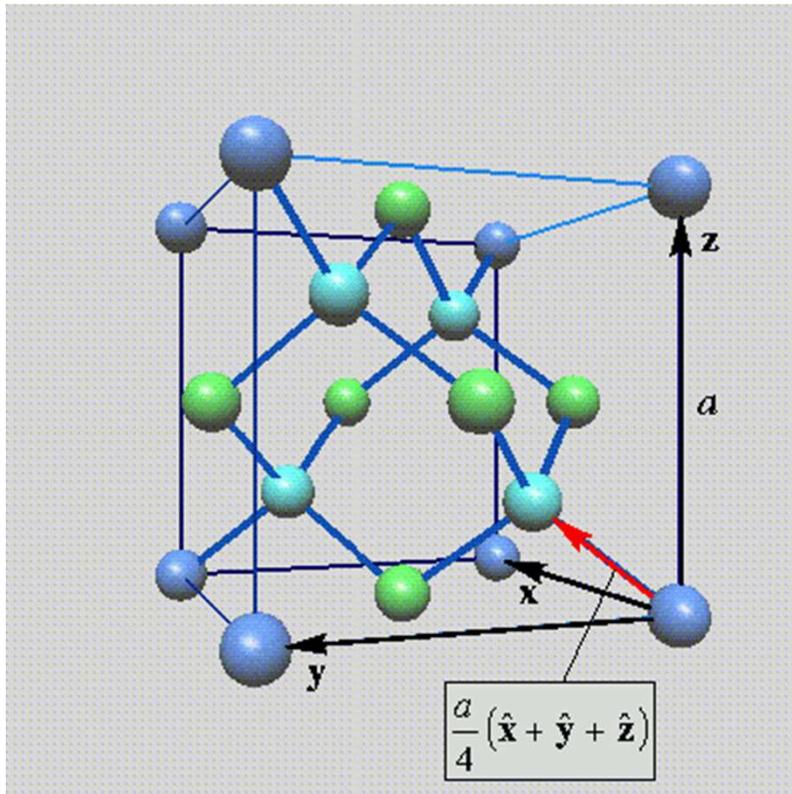
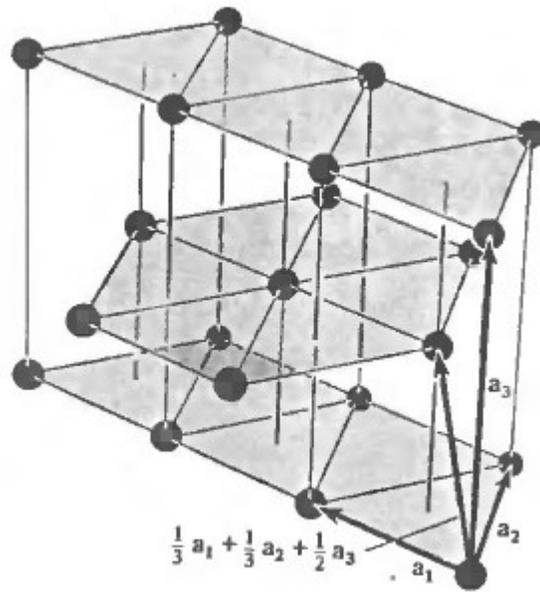


Table 4.3  
ELEMENTS WITH THE DIAMOND CRYSTAL  
STRUCTURE

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

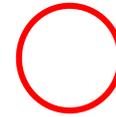
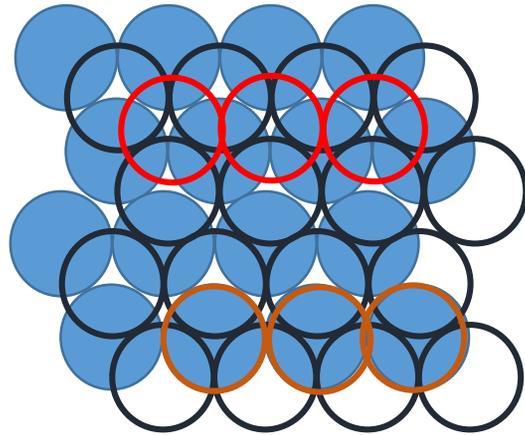


## Reticolo esagonale compatto (HCP)

**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
$\alpha$ -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

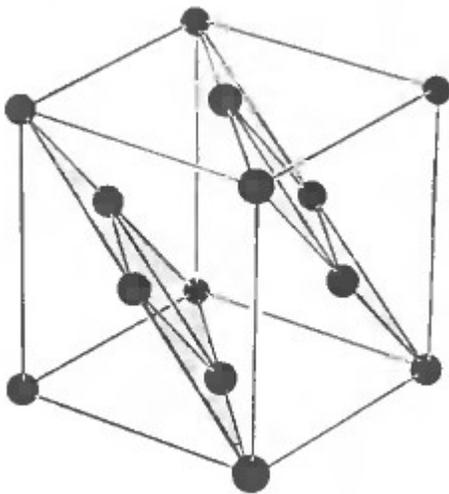
# Reticoli Close-Packed



Stacking ABC



Stacking ABAB

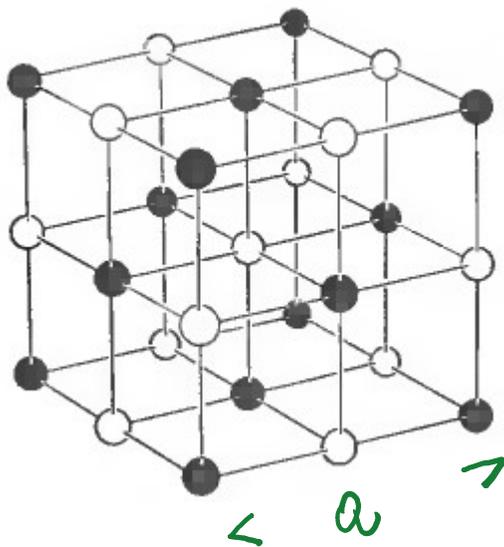


Lo stacking ABC è il reticolo FCC.

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

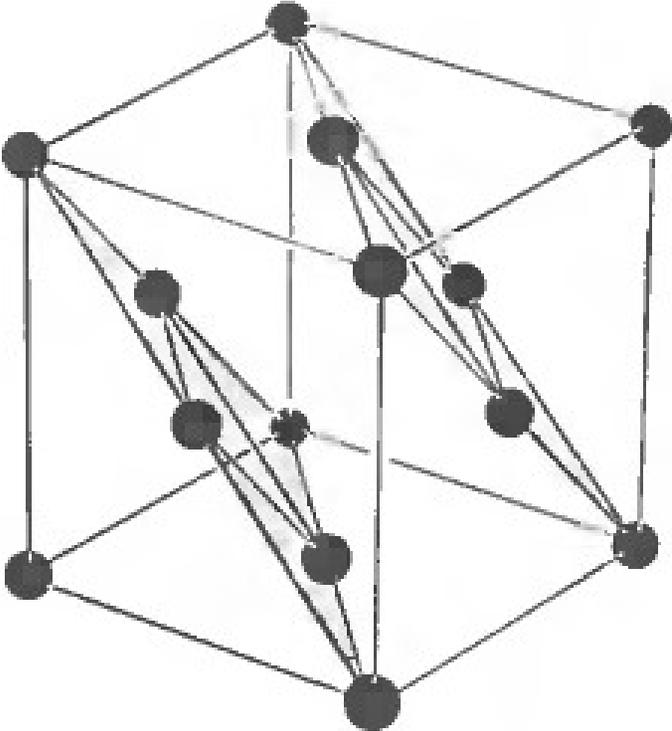
Packing : 74% (BCC: 68% SC: 52%)

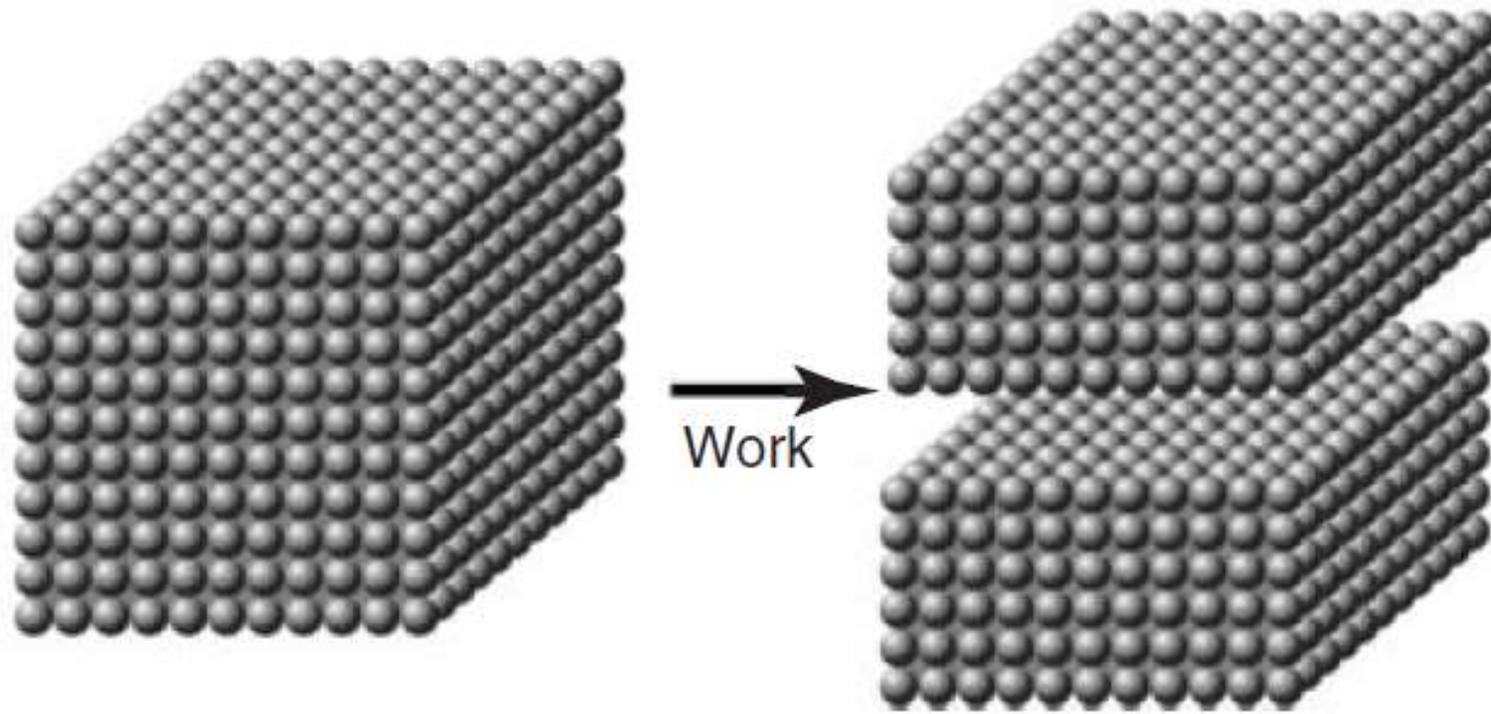
Cristalli di composti di due o più elementi sono necessariamente descritti da un reticolo con base



**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		

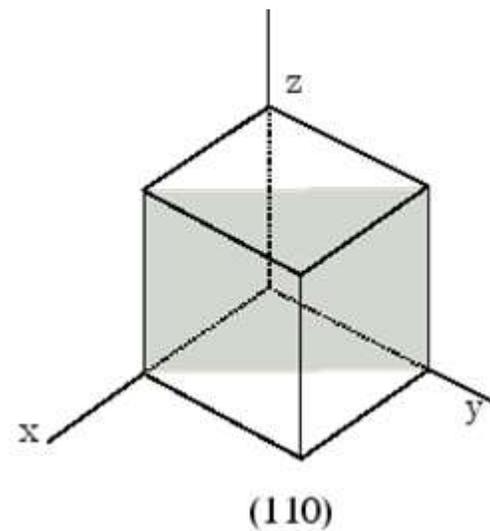
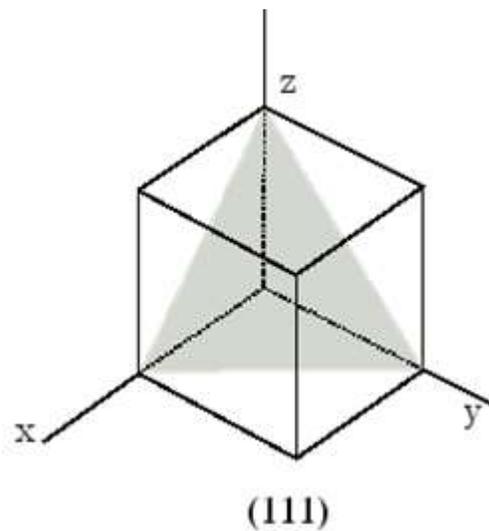
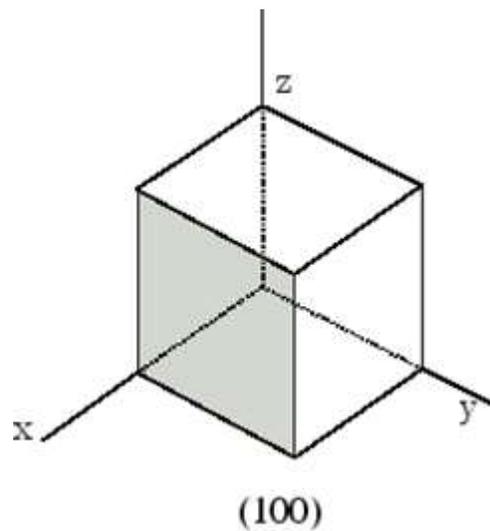
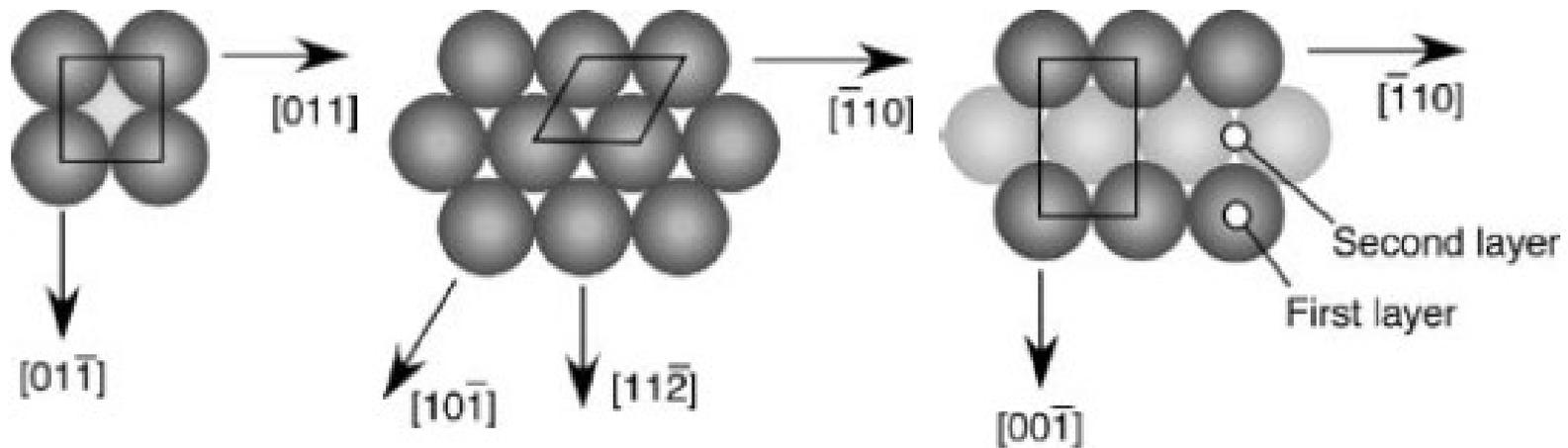




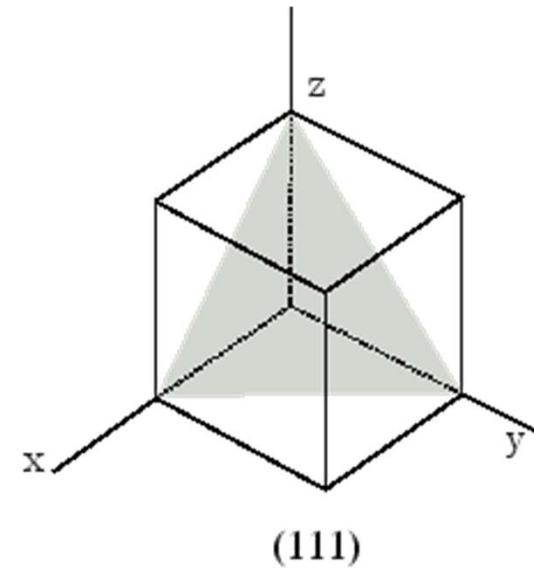
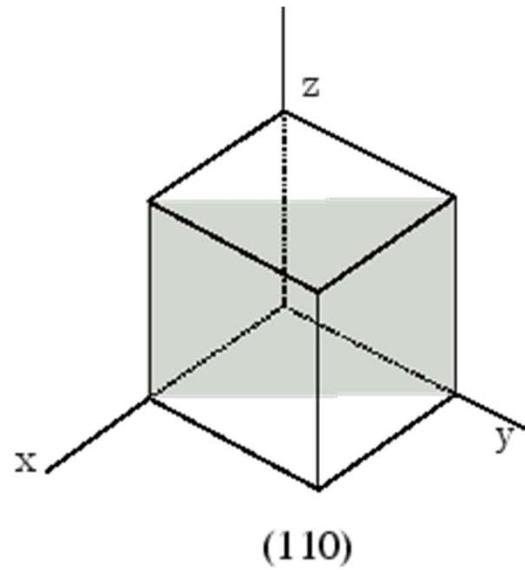
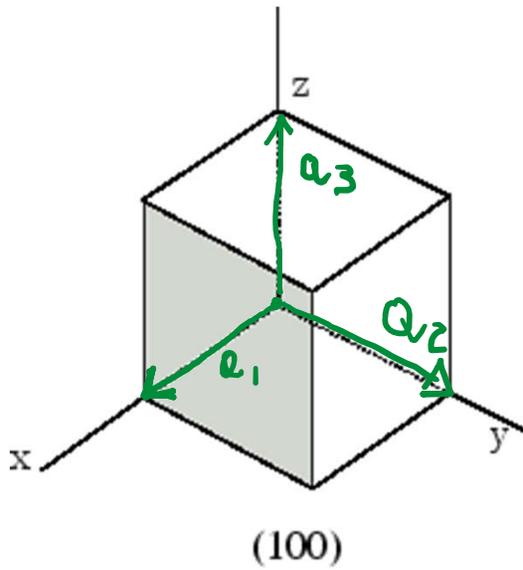
Crystal

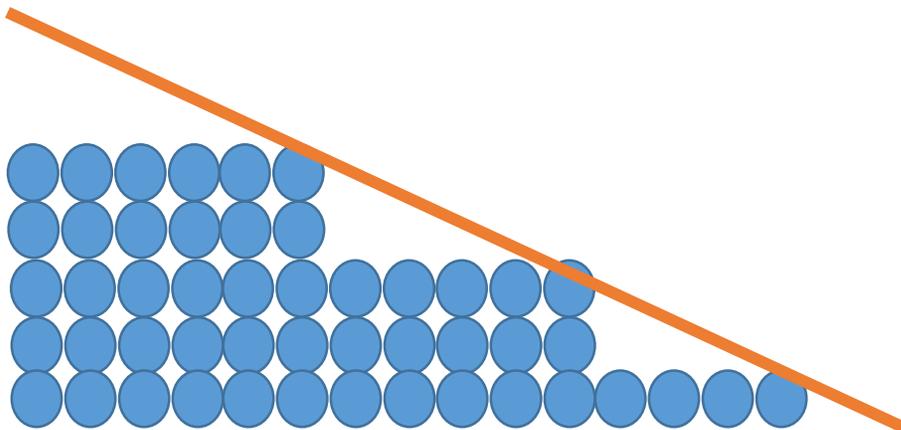
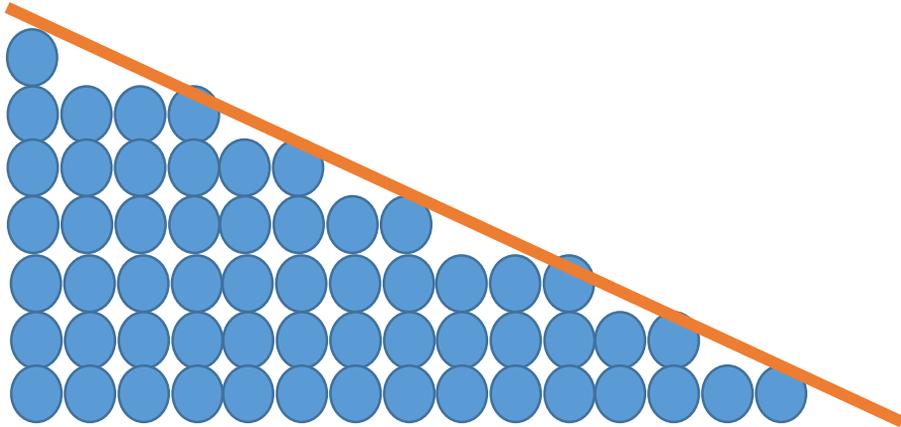
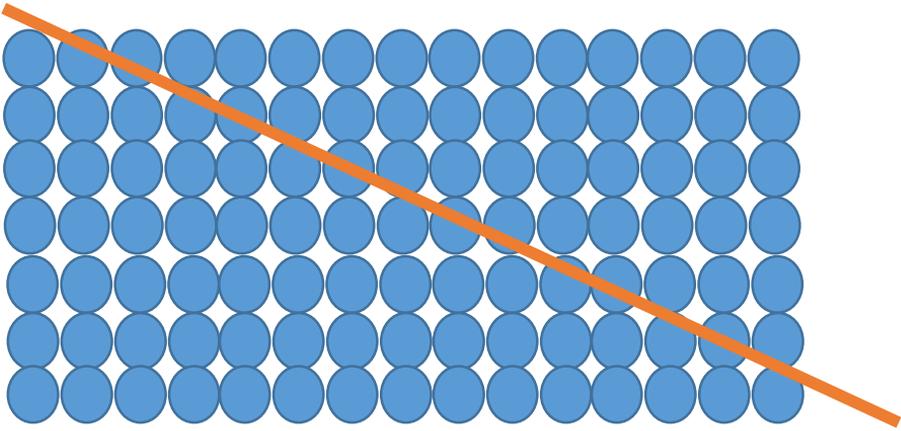
Creation of surface

## Tre diverse superfici FCC

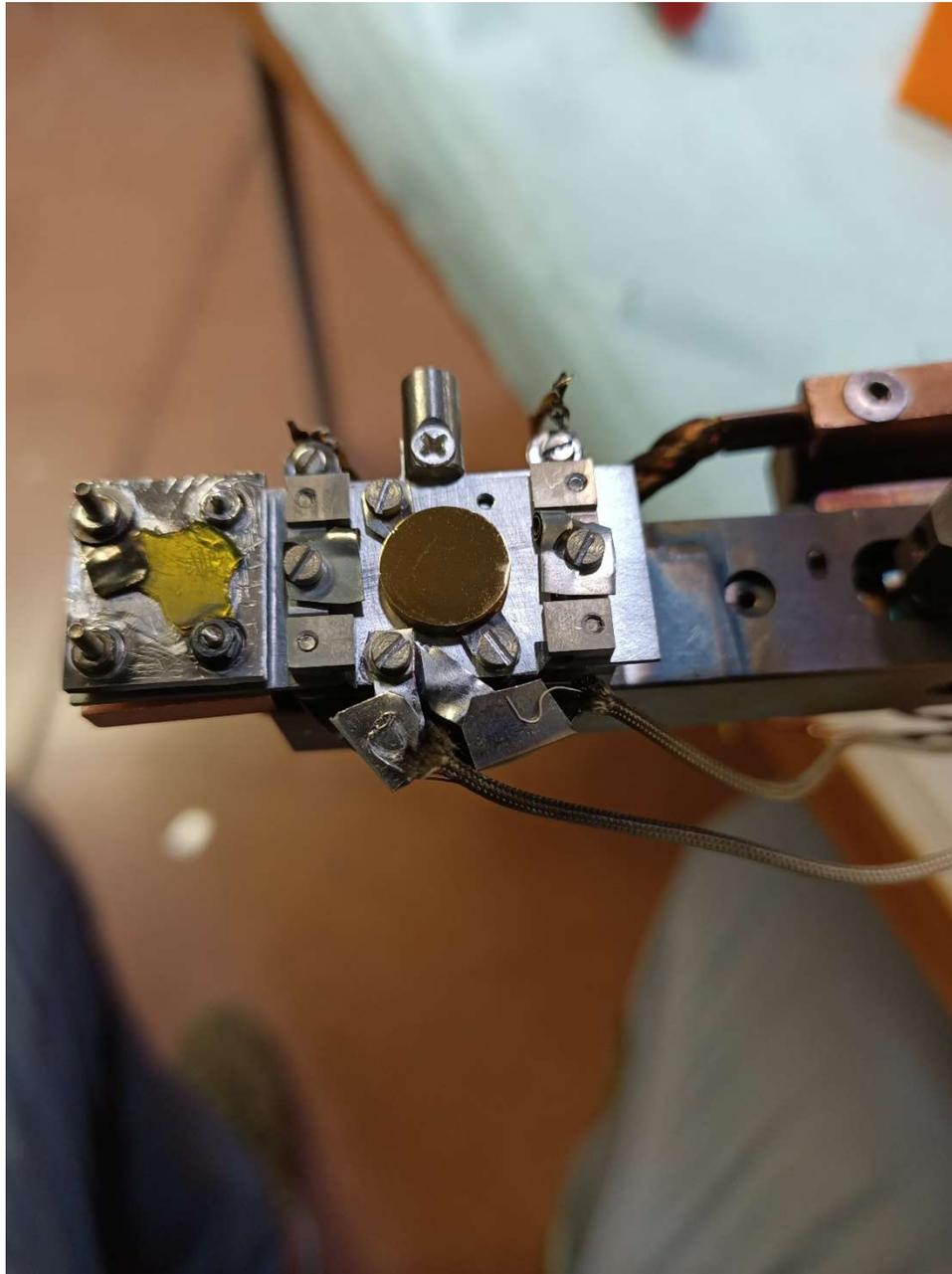


# Indici di Miller



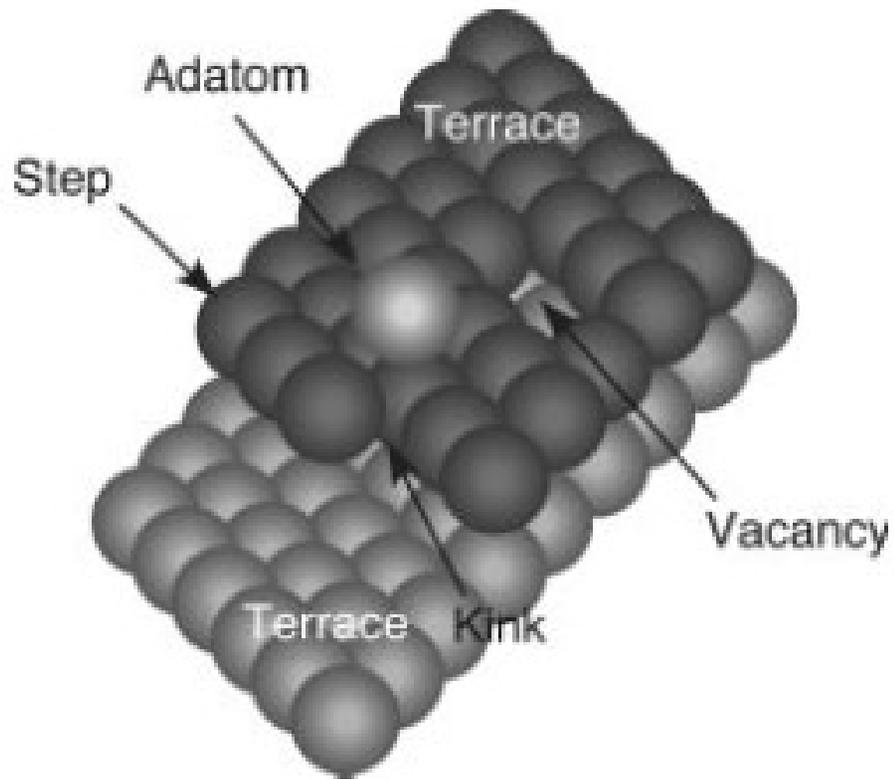


Faceting



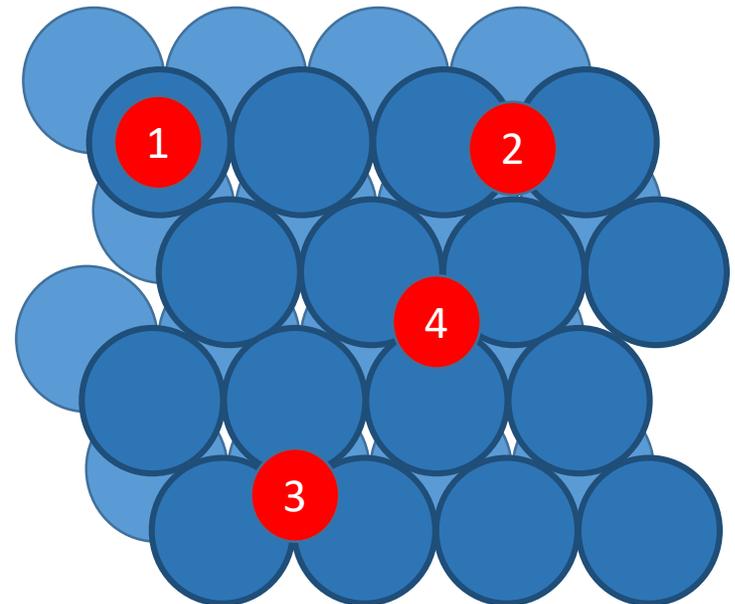
Campione di Au(111)  
Single crystal

Montaggio su portacampioni  
per misure di spettroscopia

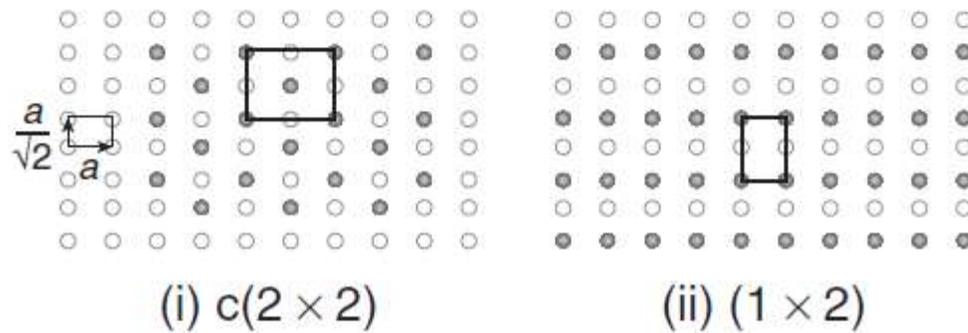
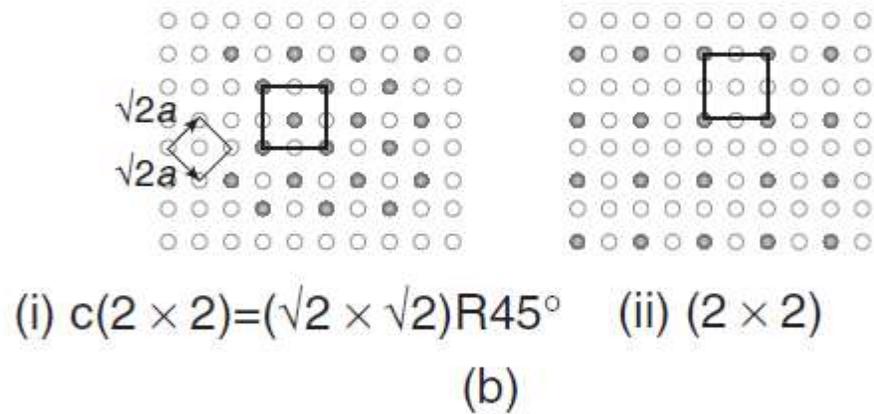
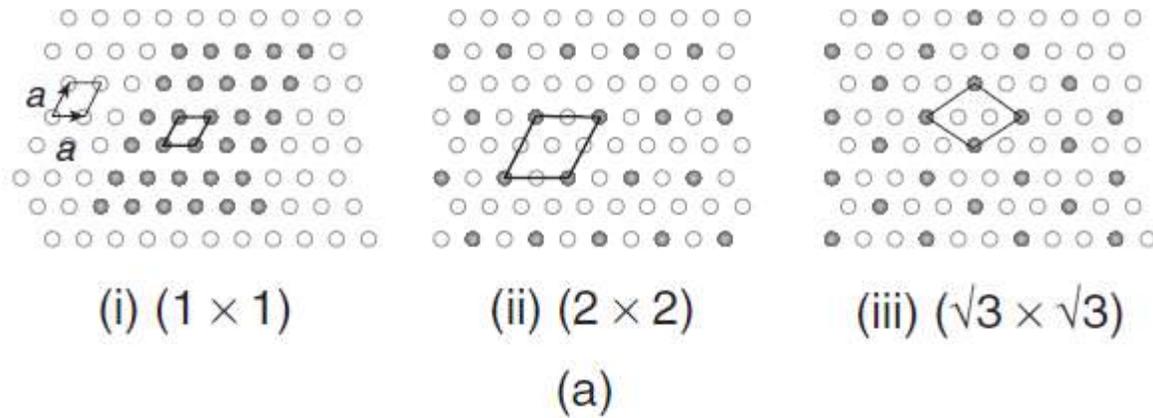


### Siti di adsorbimento:

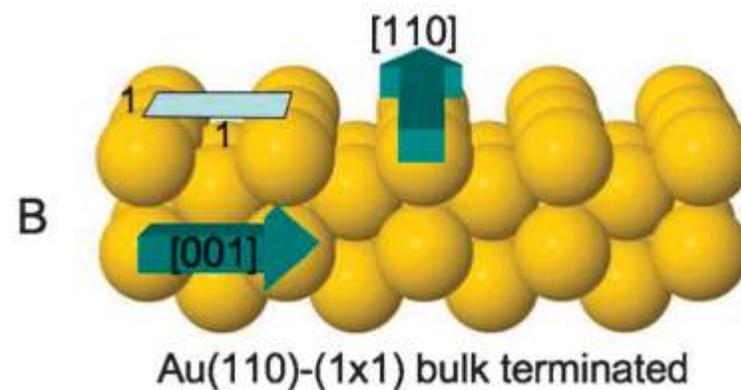
1. On Top
2. Bridge
3. Hollow HCP
4. Hollow FCC



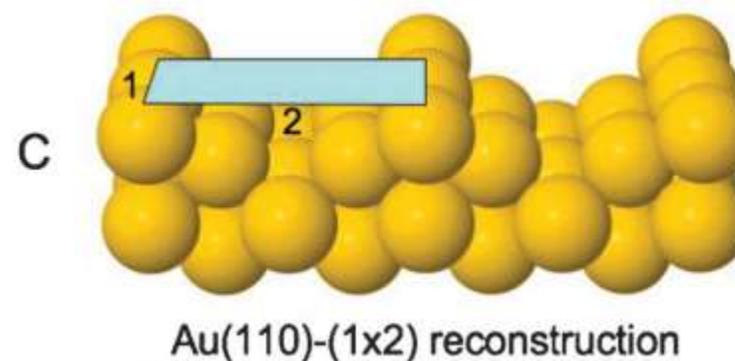
## Esempi di strutture commensurate con il substrato



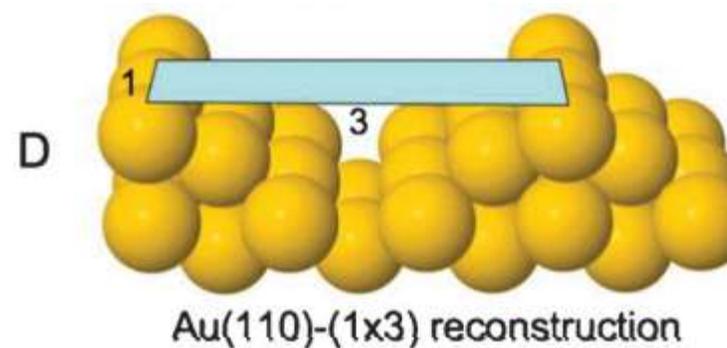
Superficie Au(110) terminata bulk  
(quella che mi aspetto semplicemente  
da un taglio del cristallo)



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



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



modes of thin-film growth

