SUPER-RETICOLI (SUPERLATTICE)

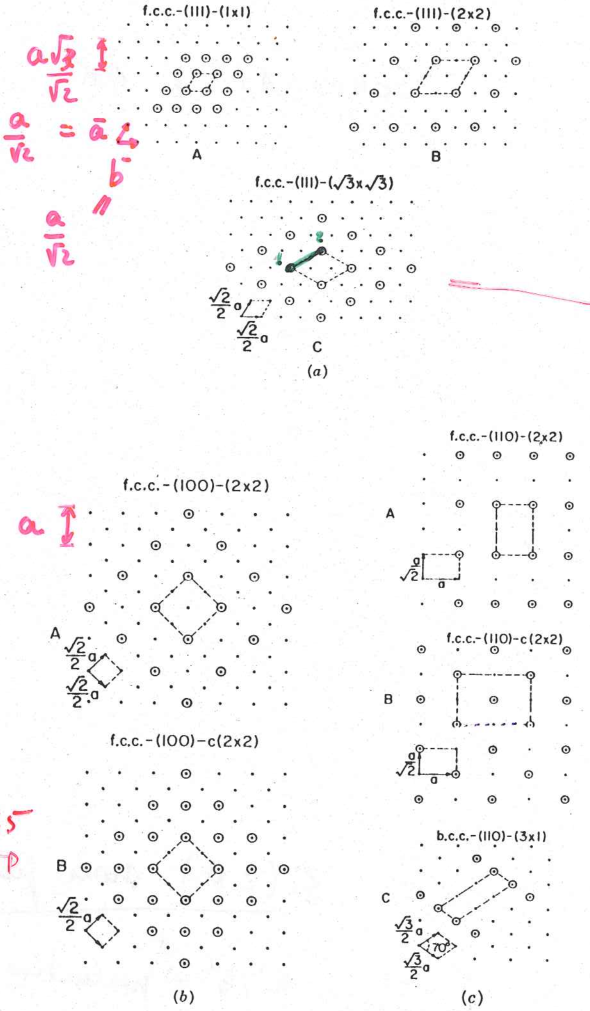


Figure 2.9. Commonly observed unit cells of adsorbate surface structures on (a) the fcc(111) crystal face, (b) the fcc(100) crystal face, and (c) the fcc(110) crystal face.

$(\sqrt{2}\times\sqrt{2})R45 \rightarrow$

A: $M = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ $\quad \bar{a}' = \bar{a}$, $\bar{b}' = \bar{b}$ $\quad (1\times1)$

B: $M = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$ $\quad \bar{a}' = 2\bar{a}$, $\bar{b}' = 2\bar{b}$ $\quad (2\times2)$

C: $M = \begin{pmatrix} 1 & 1 \\ -1 & 2 \end{pmatrix}$ $\quad \bar{a}' = \bar{a}+\bar{b}$, $\bar{b}' = -\bar{a}+2\bar{b}$

$$1\text{-}2: \sqrt{\left(\frac{1}{2}\sqrt{\frac{3}{2}}\,a\right)^2 + \left(\frac{3}{2}\frac{a}{\sqrt{2}}\right)^2} = \sqrt{\frac{3}{2}}\,a$$

$\rightarrow |a'| = \sqrt{\frac{3}{2}}\,a$ $\qquad \frac{|a'|}{|a|} = \sqrt{3}$

$|a| = \frac{a}{\sqrt{2}}$

$\Downarrow$

C: $(\sqrt{3}\times\sqrt{3})\underbrace{R30^\circ}$

$\downarrow$

Rotazione di 30°

Pt (111) (1×1)

Si (111) (1×1)-O $\quad$ Ricostruzione O/Si(111) con struttura (1×1)

Si (111) (7×7) + H $\Rightarrow$ Si (111) (1×1)+H [(1×1):H)

TABLE 2.1. (Abbreviated) and Matrix Notations for a Variety of Superlattices on Low-Miller-Index Crystal Surfaces

	Superlattice Unit Cell	
Substrate	Abbreviated Notation	Matrix Notation
fcc(100), bcc(100)	p(1 × 1)	$\begin{vmatrix}1 & 0\\0 & 1\end{vmatrix}$
	c(2 × 2) = ($\sqrt{2}$ × $\sqrt{2}$)$R45°$	$\begin{vmatrix}1 & -1\\1 & 1\end{vmatrix}$
	p(2 × 1)	$\begin{vmatrix}2 & 0\\0 & 1\end{vmatrix}$
	p(1 × 2)	$\begin{vmatrix}1 & 0\\0 & 2\end{vmatrix}$
	p(2 × 2)	$\begin{vmatrix}2 & 0\\0 & 2\end{vmatrix}$
	(2$\sqrt{2}$ × $\sqrt{2}$)$R45°$	$\begin{vmatrix}2 & 2\\-1 & 1\end{vmatrix}$
fcc(111) (60° between basis vectors)	p(2 × 1)	$\begin{vmatrix}2 & 0\\0 & 1\end{vmatrix}$
	p(2 × 2)	$\begin{vmatrix}2 & 0\\0 & 2\end{vmatrix}$
	($\sqrt{3}$ × $\sqrt{3}$)$R30°$	$\begin{vmatrix}1 & 1\\-1 & 2\end{vmatrix}$
fcc(110)	p(2 × 1)	$\begin{vmatrix}2 & 0\\0 & 1\end{vmatrix}$
	p(3 × 1)	$\begin{vmatrix}3 & 0\\0 & 1\end{vmatrix}$
	c(2 × 2)	$\begin{vmatrix}1 & -1\\1 & 1\end{vmatrix}$
bcc(110)	p(2 × 1)	$\begin{vmatrix}2 & 0\\0 & 1\end{vmatrix}$

c(2x2) → centrata (2x2)

p → primitiva

$$\begin{pmatrix}\bar{a}'\\ \bar{b}'\end{pmatrix} = \begin{pmatrix}m_{11} & m_{12}\\ m_{21} & m_{22}\end{pmatrix}\begin{pmatrix}\bar{a}\\ \bar{b}\end{pmatrix}$$

$$\bar{a}' = m_{11}\bar{a} + m_{12}\bar{b}$$

$$\bar{b}' = m_{21}\bar{a} + m_{22}\bar{b}$$

STRUTTURA A DIAMANTE (Si, Ge) O ZINCOBLENDA (GeAs)

BULK

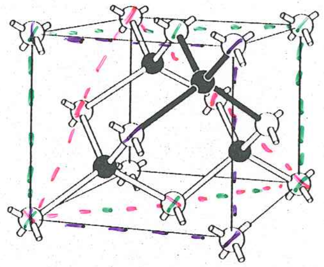
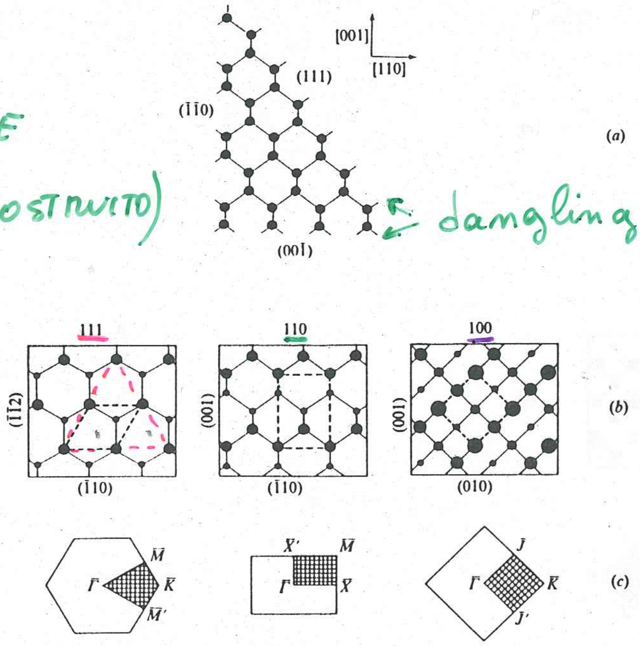


Fig. 6.1. Ball-and-stick model of the zincblende atomic geometry. Open circles represent cations (e.g., Zn) and closed circles anions (e.g., S). If both species are identical (e.g., C, Si, Ge), then this structure becomes the diamond atomic geometry. Balls represent atomic species and lines (i.e., "sticks") the bonds between them. The heavy shadowed lines around the second-layer atom indicate the tetrahedral coordination of the individual atomic species in these structures.

Fig. 4.35. Crystallography of a homopolar semiconductor: (*a*) edge view that illustrates the ideal termination of three low-index faces (Harrison, 1980); (*b*) top view – decreasing atom size indicates increasing distance from the surface. Dashes outline the surface unit mesh; (*c*) corresponding ideal surface Brillouin zone with conventional labelling (Ivanov, Mazur & Pollmann, 1980).

CASO IDEALE (NON ricostruito)



← dangling bonds

(111) 1 dangling bond per cella unitaria (1at/cella)

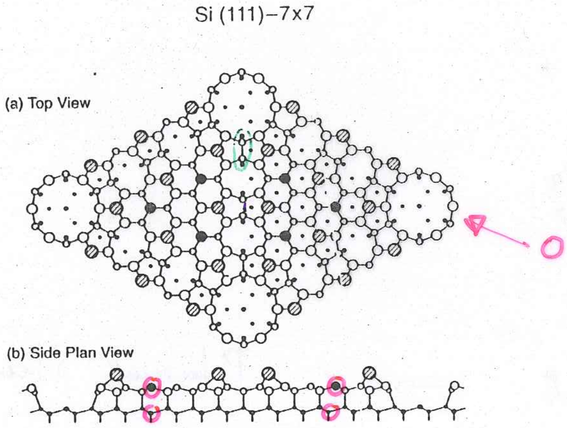
(110) 2 " " (2at/cella)

(100) 2 " " (1at/cella)

Ogni dangling bond ha 1 elettrone (semipieno)

Si (111) 7x7

FAULTED ←|→ UNFAULTED



STACKING FAULT (DIFETTO DI IMPILAMENTO)

Fig. 6.5. Schematic illustration of the top (panel a) and side (panel b) views of the dimer–adatom-stacking-fault (DAS) model of the Si(111)–7×7 structure. The side view is given along the long diagonal of the unit cell. In the top view (panel a) the large shaded circles designate the adatoms in the top layer of the structure. The large solid circles designate "rest atoms" in the second layer which are not bonded to an adatom. Large open circles designate triply bonded atoms in this layer, whereas small open circles designate fourfold coordinated atoms in the bilayer beneath. Smaller solid circles designate atoms in the fourth and fifth bilayers from the surface. The size of all circles is proportional to the proximity to the surface. The side view (panel b) is a plan view of nearest neighbor bonding in a plane normal to the surface containing the long diagonal of the surface unit cell. Smaller circles indicate atoms out of the plane of this diagonal. Adapted from Takayanagi et al. (1985).

▨ Adatoms 12/cella 9 dimers/cella

● REST ATOMS 6/cella 1 corner hole/cella O

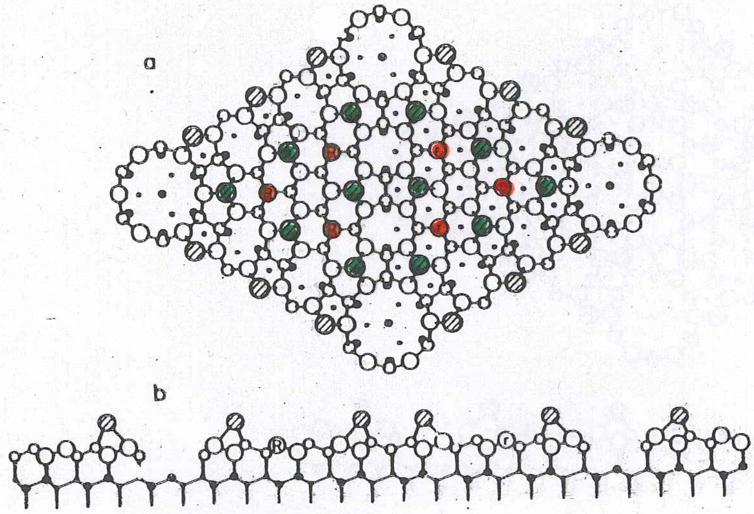
7x7 non ricostruita ⟹ 49 atomi → 49 dangling

7x7 ricostruita → 18 atomi sup./cella → 19 dangling

(18+1 dagli angoli)

12 adatoms + 6 rest atoms

Si(111) 7x7

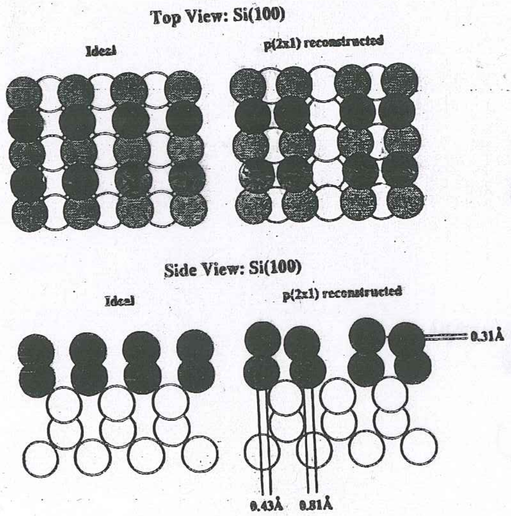


● REST ATOMS

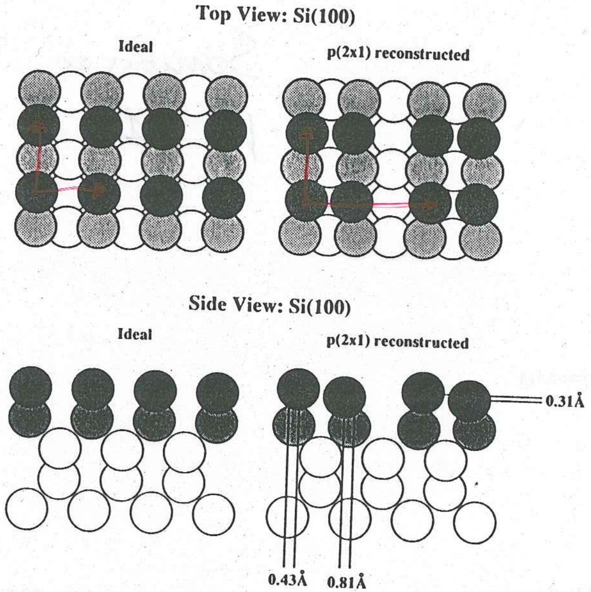
● Adatoms

19 dangling bonds

Si (100) 2x1



Si (100) 2x1


Top View: Si(100)

Ideal

p(2x1) reconstructed

Side View: Si(100)

Ideal

p(2x1) reconstructed

Figure 2.13. The reconstructed silicon (100) crystal face as obtained by LEED surface crystallography. Note that surface relaxation extends to three atomic layers into the bulk [166].

$a' = 2a$

$b' = 1b$

$M = \begin{vmatrix} 2 & 0 \\ 0 & 1 \end{vmatrix}$

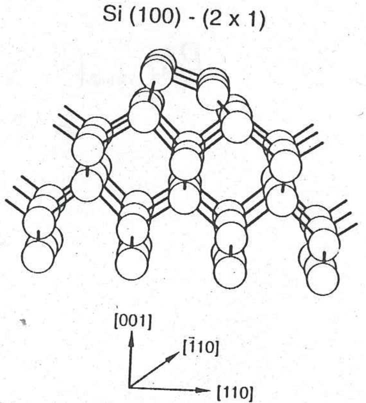

Si (100) - (2 x 1)

Fig. 6.6. Ball-and-stick model of the buckled dimer structure of Si(100)(2×1). Adapted from MacLauren et al. (1987).

Si (111) 2x1

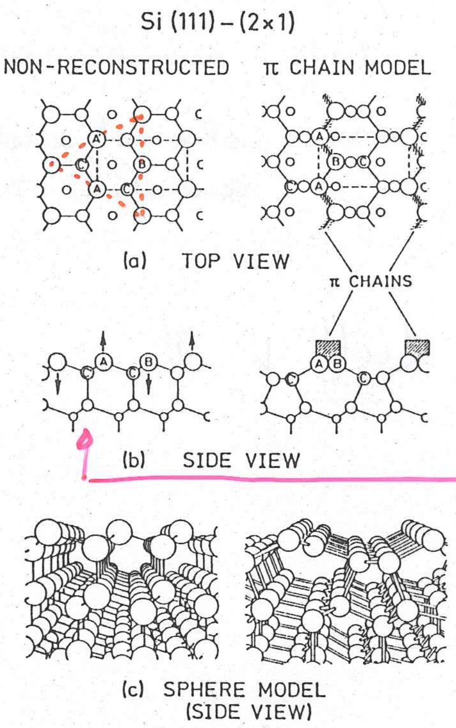
SI OTTIENE DA CLEAVED Si (111) IN UHV

Si (111) cleaved (T≤300-400°C) 2x1

Si (111) cleaved (400<T<800°C) 7x7

annealed (T~1100°C) 7x7

Si (111) cleaved at T>800°C 1x1



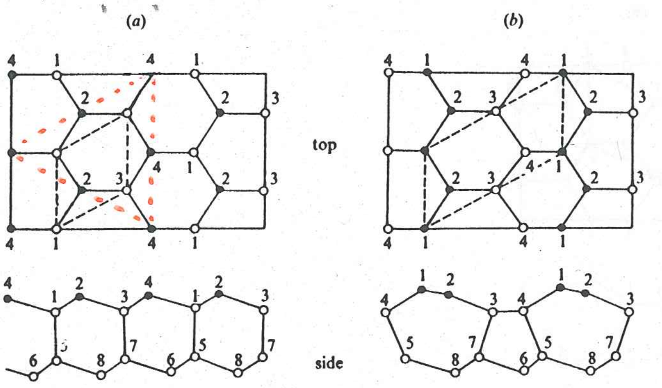
π - BONDED CHAIN MODEL OK

buckling MODEL (NO BUONO!)

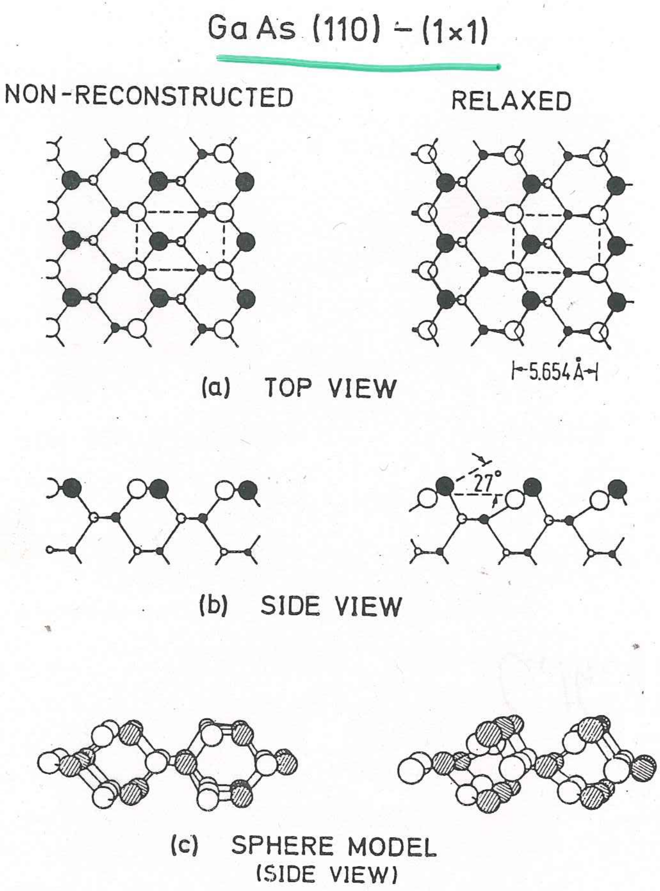
CATENA ZIG-ZAG (CHAIN)

Fig. 3.6a-c. Atomic positions at the Si(111) surface; ideal, non-reconstructed and with (2 × 1) reconstructuion (π-bonded chain model) as occurs after cleavage in UHV. The shaded areas denote the location of the chains originating from overlap between neighboring dangling bonds. (a) Top view, the (2 × 1) unit mesh is plotted in broken line. (b) Side view; arrows indicate possible up- and downwards shifts of surface atoms of type A and B, which give rise to the so-called buckling reconstruction. (c) Sphere model. (*Smaller circles* indicate deeper atomic layers)

Fig. 4.40. Top and side view of Si(111): (*a*) ideal surface; (*b*) π-bonded chain model. Dashes outline the surface unit cells and shaded circles identify the surface atoms that 'dangle' $3p_z$ orbitals into the vacuum (Pandey, 1981).



RILASSAMENTO NEI SEMICONDUTTORI SENZA RICOSTRUZIONE → (1×1)



○ Ga
● As

Fig. 3.5a-c. Atomic positions of the GaAs(110) surface; ideal, non-reconstructed and relaxed as it appears after cleavage in UHV. (a) Top view; the (1 × 1) unit mesh is plotted as a broken line. (b) Side view. (c) Sphere model. (*Open circles* designate Ga atoms and *shaded circles* As. *Smaller circles* indicate deeper atomic layers)

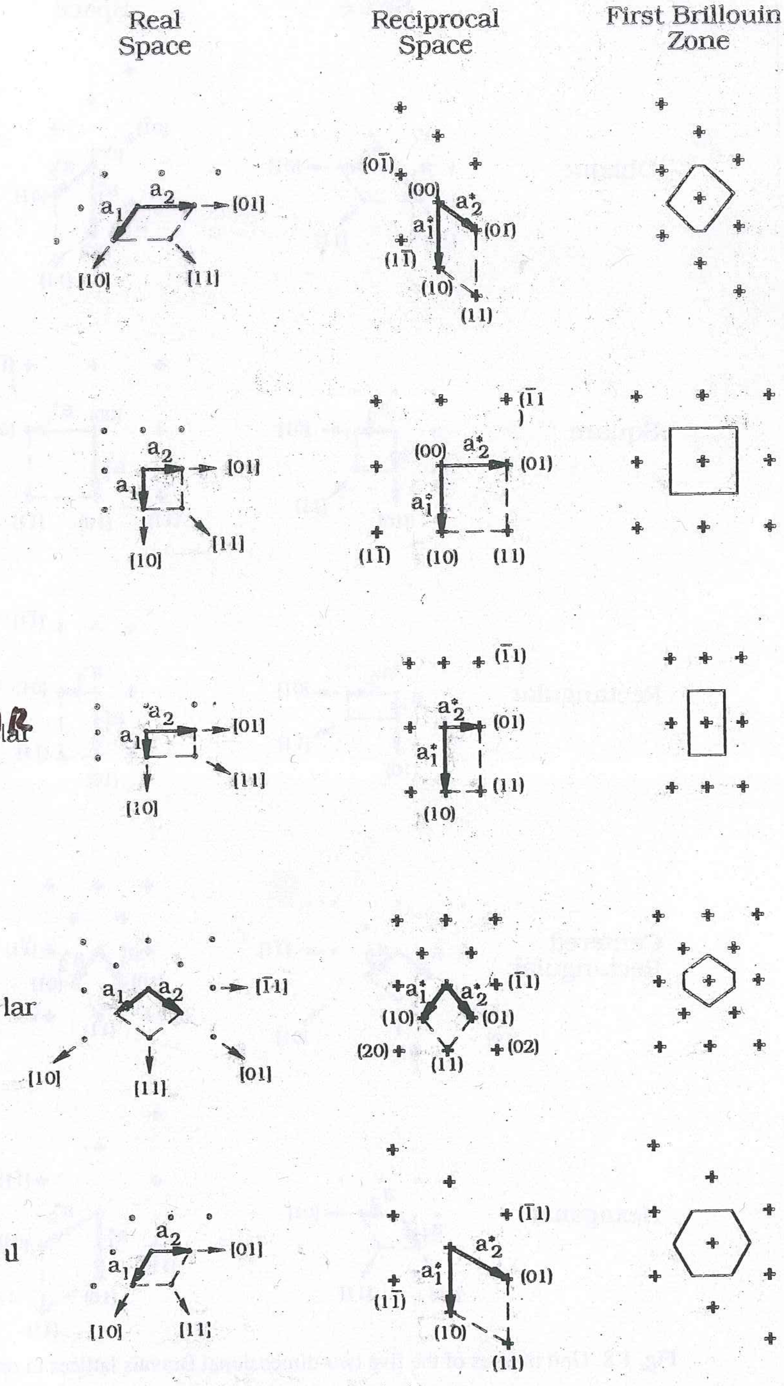
OBLIQUE
$a_1 \neq a_2$
$\gamma \neq 90°$

SQUARE
$a_1 = a_2$ $\gamma = 90°$

RECTANGULAR
$a_1 \neq a_2$ $\gamma = 90°$

CENTERED
RECTANGULAR

HEXAGONAL
$a_1 = a_2$
$\gamma = 120°$



ımeshes of the five two-dimensional Bravais lattices in real and reciprocal spaces.

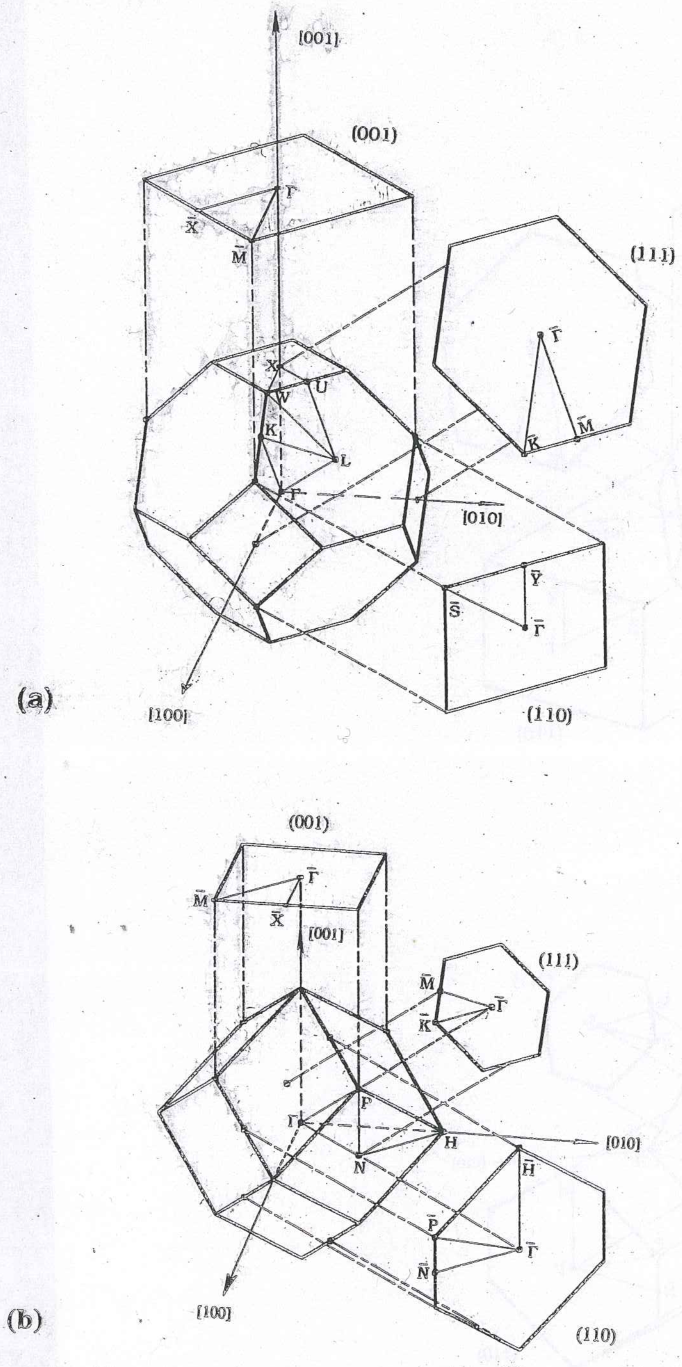


Fig. 1.13. (a) First Brillouin zones for the bulk, (111), (110), and (001) planes of fcc crystals. (b) First Brillouin zones for the bulk, (111), (110), and (001) planes of bcc crystals. (Reproduced with permission of W.N. Unertl.)

Surface (100) → [100] [illegible]

FCC LATTICE

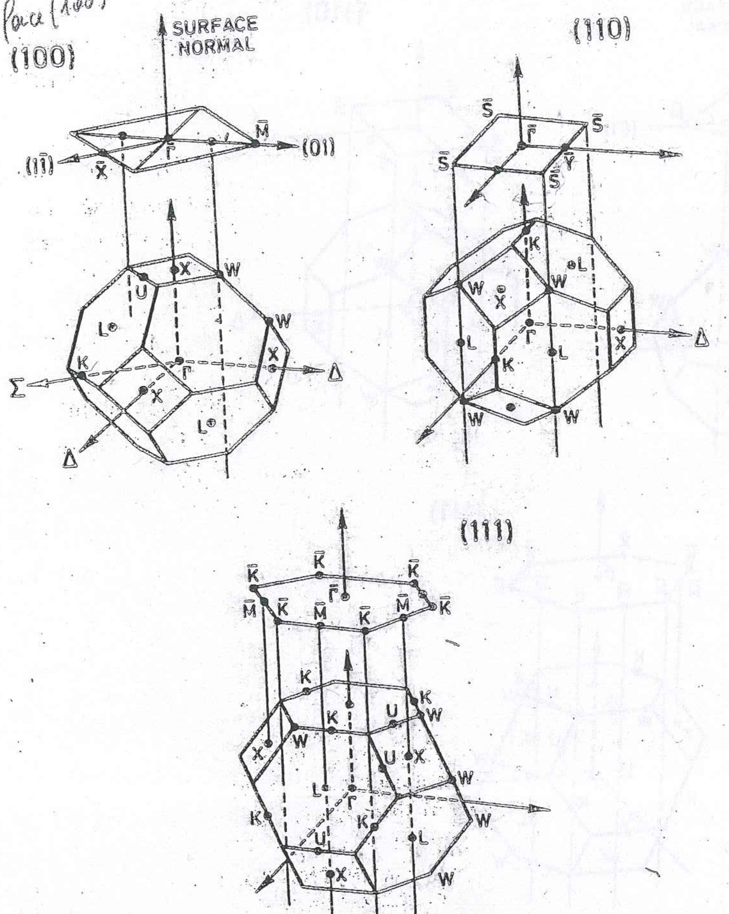


Fig.5.5. Relation between the 2D surface Brillouin zones of the (100), (111) and (110) surfaces of a fcc lattice and the bulk Brillouin zone

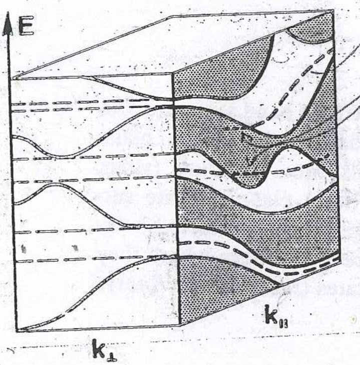


Fig.6.4. Hypothetical electronic band structure of a crystal. The shaded areas in the $E(k_\parallel)$ plane describe the projected bulk-band structure (along $k_\perp$). Broken lines in the $E(k_\parallel)$ plane indicate surface state bands in the gaps of the projected bulk-band structure, and surface resonances where they are degenerate with bulk states (*short dotted lines*)

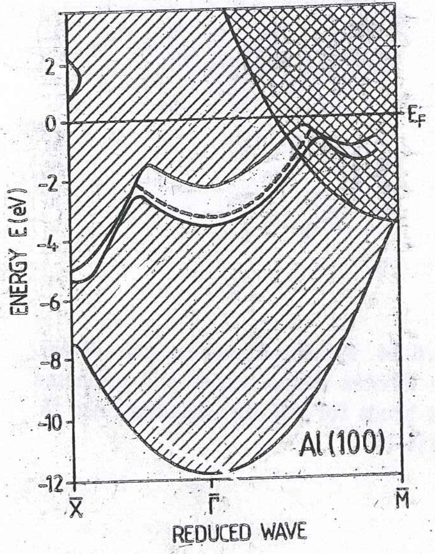
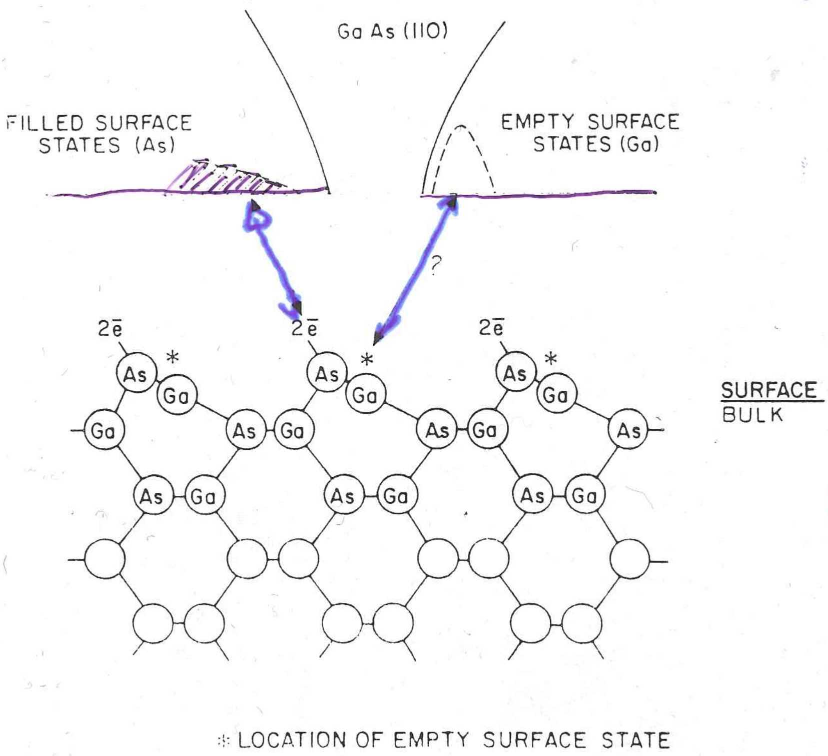


Fig.6.14. Measured surface state dispersion (*broken curve* [6.13]) and projected bulk bands for Al(100) (*shaded area* [6.15]) [6.14]

- Non tutti i semicond. hanno stati di superficie nella Gap → no band bending

Es. GaAs (110)



1) Rottura legame in superficie
↓
Ga e As atomici
↓
stati nella gap

2) Ricostruzione
↓
shift fuori gap

Fig. 1. The GaAs (110) surface. Both the electronic and atomic surface rearrangements are indicated. (From ref. 17)

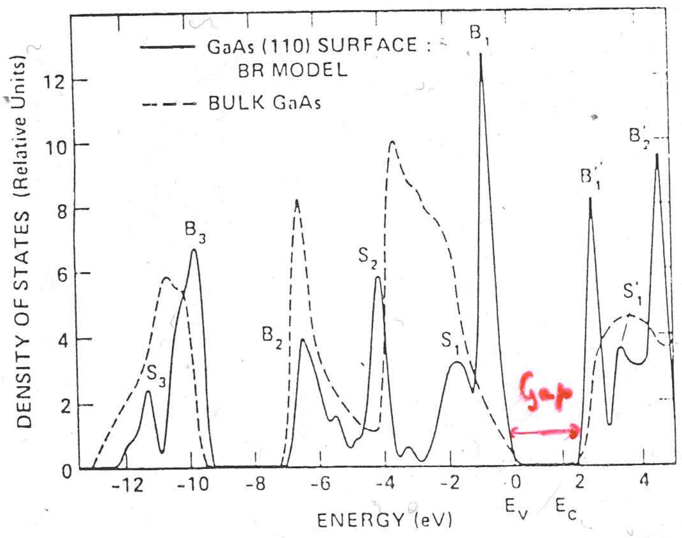


Fig. 2. The local density of states (solid line) for the bond-relaxation model of the (110) surface of GaAs. (From ref. 59)