

SUPERFICIE: DIFETTI E RILASSAMENTO

- DIFETTI

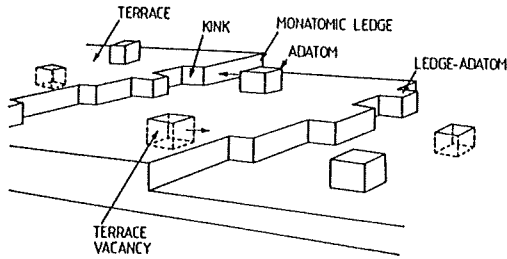


Fig. 3.8. Schematic drawing of various defects that may occur on a solid surface

- VACANZE DI UNA SINGOLA SPECIE ATOMICA (es. Ga in GaAs)
- DIFETTI ANTI-SITO (Ga al posto di As)
- STEP MONOATOMICI CON MOLTI LEGAMI PENDENTI (DANGLING BONDS)

- RILASSAMENTO E RICOSTRUZIONE

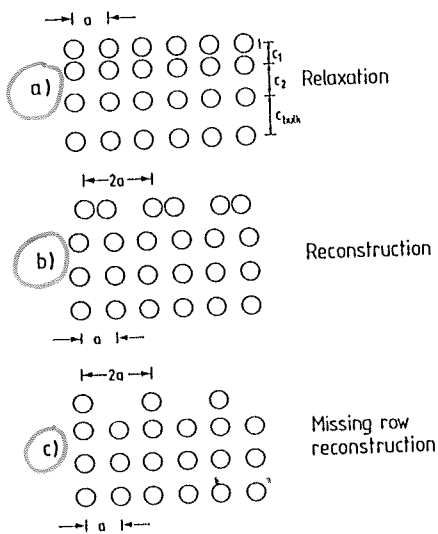


Fig. 3.4a-c. Schematic side view of the characteristic rearrangements of surface atoms of a simple cubic lattice with lattice constant a : (a) Relaxation of the topmost atomic layer normal to surface (different lattice spacings c); (b) reconstruction of the topmost atomic layer into a surface net with double periodicity distance $2a$; (c) missing row reconstruction with missing atoms in the topmost lattice plane

a) Rilassamento:
 2D superficiale =
 2D bulk -
 Solo compressione o
 espansione verticale
 stretto (es. -10% Cu (110),
 -10% Al (110),
 0% Cu (100))

b) RICOSTRUZIONE:
 2D superficiale \neq 2D bulk

c) Ricostruzione con "scomparsa"
 di atomi superficiali

RICOSTRUZIONI MOLTO PIU' FREQUENTI NEI
 SEMICONDUCTORI CHE NEI METALLI PER EFFETTO
 DEI LEGAMI DIREZIONATI

SUPERFICIE

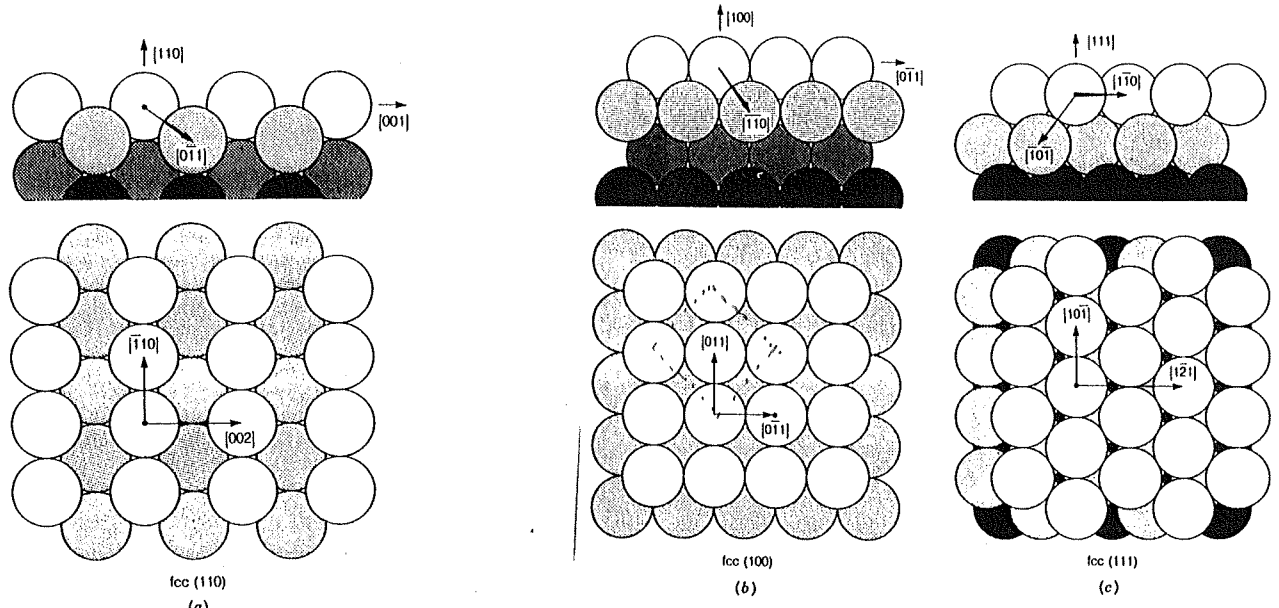
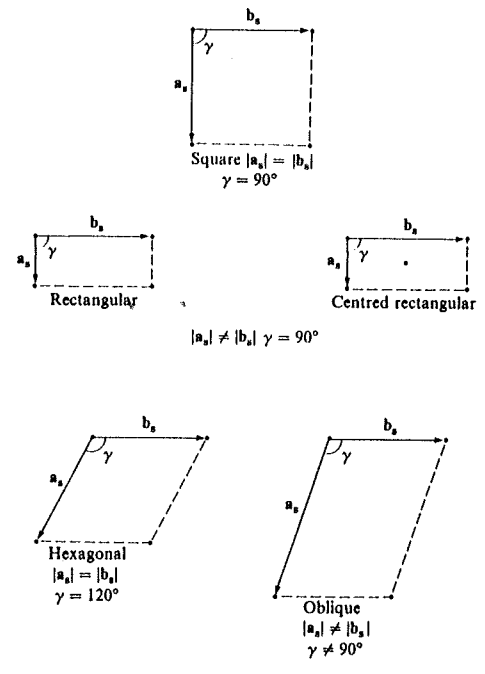


Figure 2.8. Top views and side views of the face-centered cubic (fcc) crystal surfaces: (a) (110), (b) (100), and (c) (111)

Figure 2.8. (Continued)

Fig. 3.3. The five surface nets (Pruitt, 1983).



2D

\bar{a}, \bar{b} vettori della unitaria bulk (proiezione)

\bar{a}', \bar{b}' vettori della unitaria superficie

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

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

$$M = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}$$

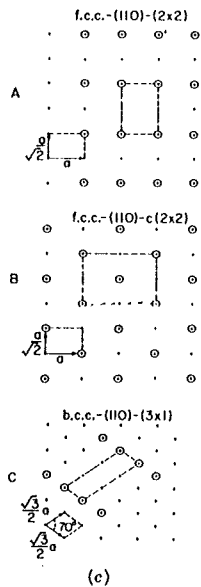
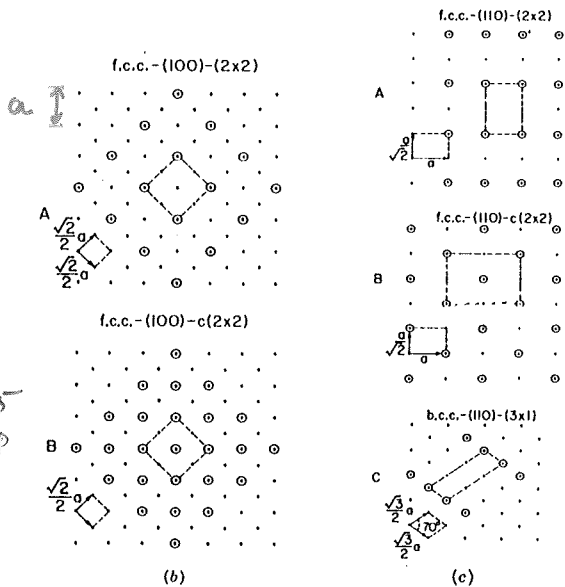
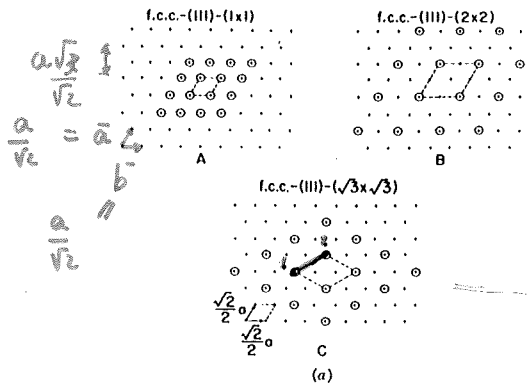
$$M = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \text{ nei tre casi sopra FCC}$$

SUPER-RETICOLI (SUPERLATTICE)

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

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

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



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

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

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

$$\frac{|a'|}{|a|} = \sqrt{3}$$

$$C: (\sqrt{3} \times \sqrt{3}) R 30^\circ$$

Rotazione di 30°

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.

Pt (111) (1x1)

Si (111) (1x1) - O

Ricostruzione O / Si(111) con struttura (1x1)

Si (111) (7x7) + H \Rightarrow Si (111) (1x1) + H [(1x1):H]