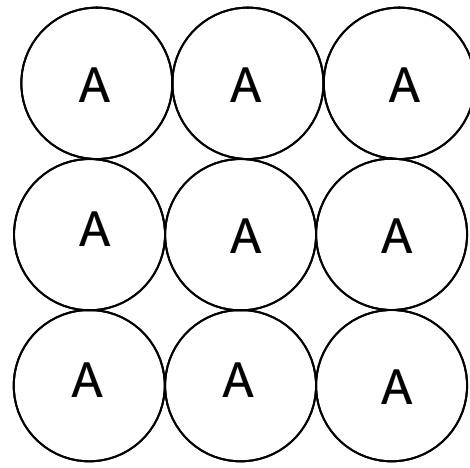


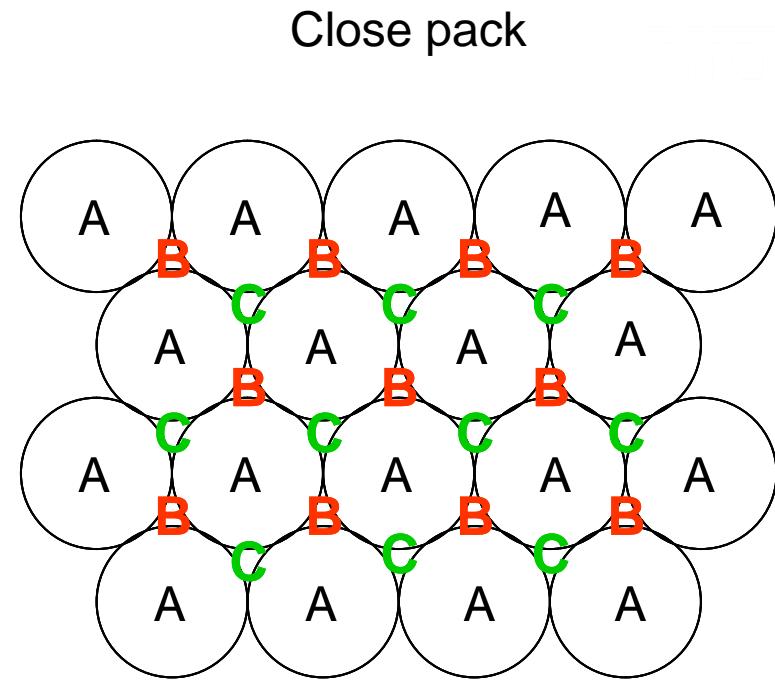
# Atomic packing density



Sequence AAAA... - simple cubic

## Atomic Packing Fraction (APF)

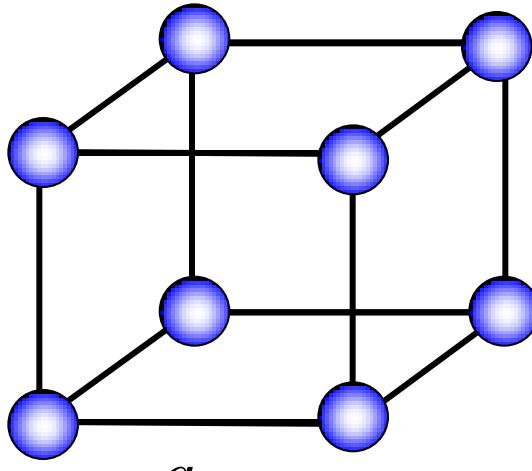
Fraction of volume in a crystal structure that is occupied by atoms.



Sequence ABABAB... - hexagonal close pack

Sequence ABCABCAB... - face centered cubic close pack

# Simple Cubic (SC) lattice



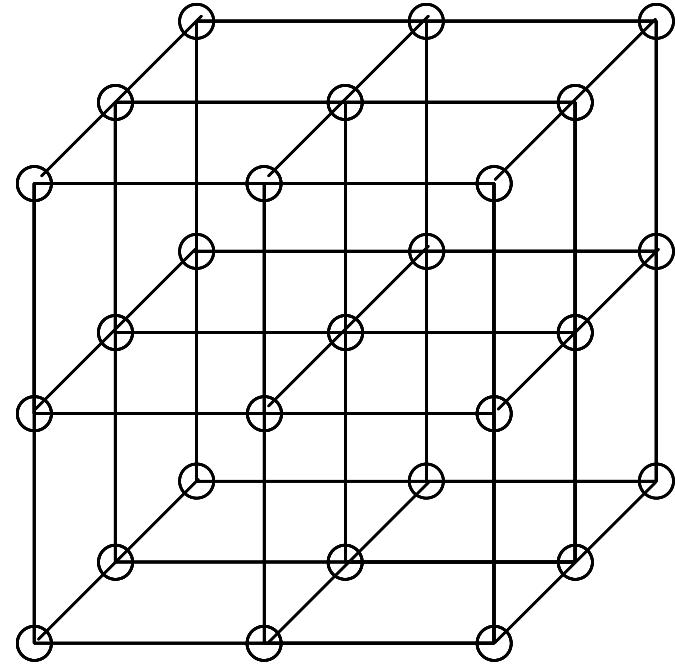
$a$  -lattice parameter

Packing fraction(packing density) =

$$= \frac{\text{No. of atoms} \times \text{Vol. of atom}}{\text{Vol. of unit cell}} = \frac{1 \times \frac{4}{3} \pi R^3}{a^3}$$

$$\text{Packing Fraction} = \frac{\pi}{6} = 0.52$$

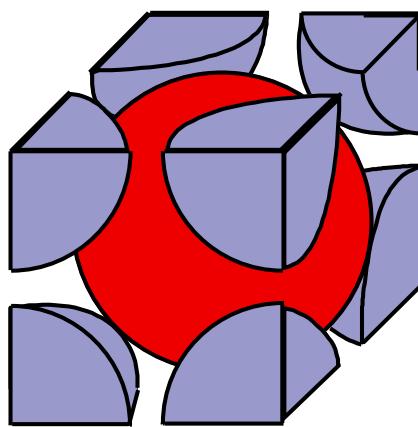
8 corner atoms shared by 8 cells →  
**1 atom per unit cell**



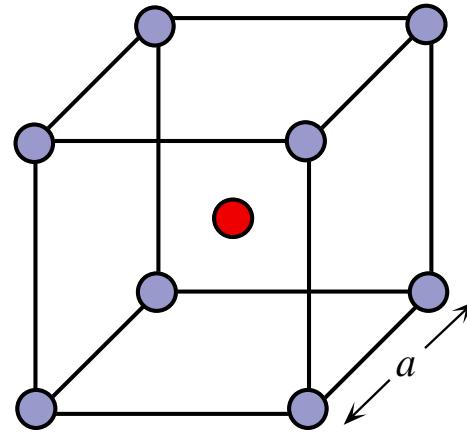
The **coordination number** represents the number of nearest-neighbor or touching atoms within the unit cell.

# Body Centered Cubic (BCC) lattice

8 corner atoms shared by 8 cells + one centered atom → **2 atoms per cell**



a



b

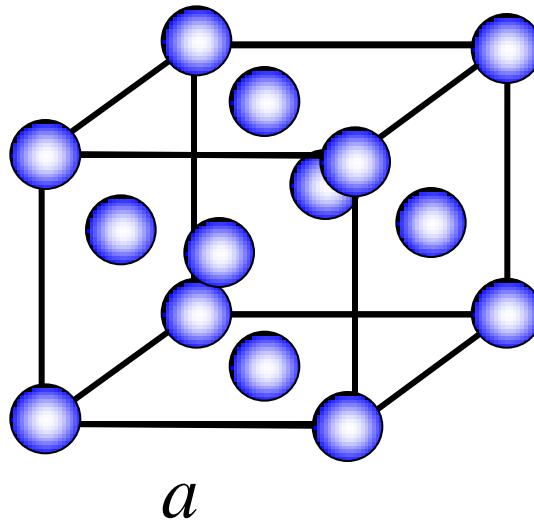
$$\text{Packing fraction} = \frac{\sqrt{3}}{8} \pi$$

Examples: Alkali metals (Li, Na, K, Rb), Cr, Mo, W, Mn,  $\alpha$ -Fe (< 912°C),  $\beta$ -Ti (> 882°C).

Fig. 1.31: Body centered cubic (BCC) crystal structure. (a) A BCC unit cell with closely packed hard spheres representing the Fe atoms. (b) A reduced-sphere unit cell.

From *Principles of Electronic Materials and Devices, Second Edition*, S.O. Kasap (© McGraw-Hill, 2002)  
<http://Materials.Usgask.Ca>

# Face Centered Cubic (FCC) lattice



$$\text{Packing fraction} = \frac{\sqrt{2}}{6} \pi$$

8 corner atoms shared by 8 cells + 6 face-centered atoms each shared by two cells  
→ **4 atoms per cell**

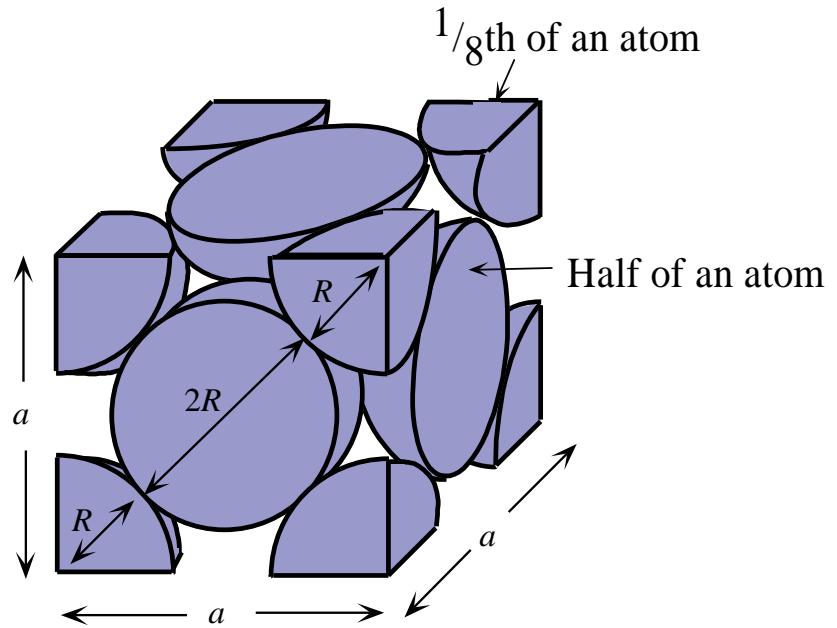


Fig. 1.38: The FCC unit cell. The atomic radius is  $R$  and the lattice parameter is  $a$

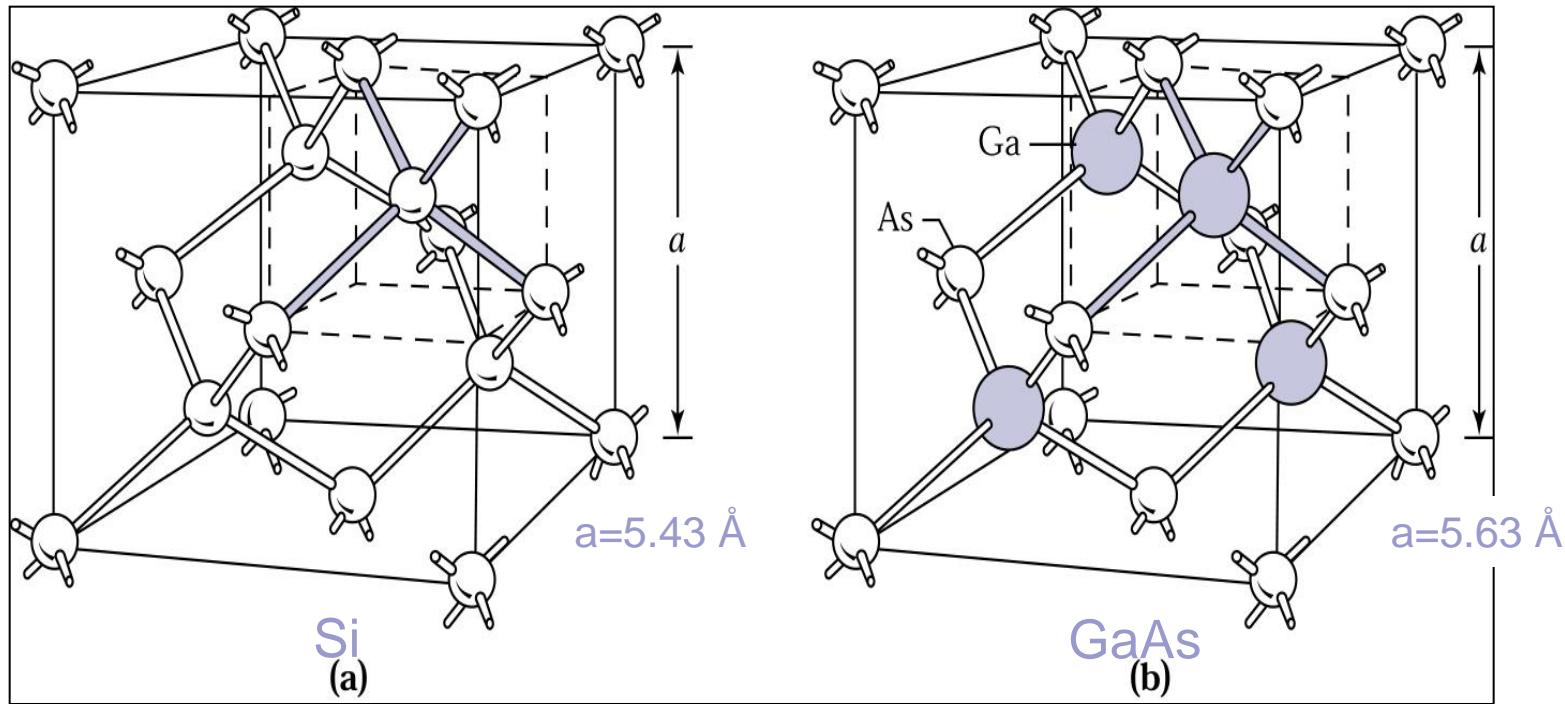
# Properties for some crystal structures

	Simple	Body-centered	Face-centered
Volume, conventional cell	$a^3$	$a^3$	$a^3$
Lattice points per cell	1	2	4
Volume, primitive cell	$a^3$	$\frac{1}{2}a^3$	$\frac{1}{4}a^3$
Lattice points per unit volume	$1/a^3$	$2/a^3$	$4/a^3$
Number of nearest neighbors <sup>a</sup>	6	8	12
Nearest-neighbor distance	$a$	$3^{1/2}a/2 = 0.866a$	$a/2^{1/2} = 0.707a$
Number of second neighbors	12	6	6
Second neighbor distance	$2^{1/2}a$	$a$	$a$
Packing fraction <sup>b</sup>	$\frac{1}{6}\pi$ $= 0.524$	$\frac{1}{8}\pi\sqrt{3}$ $= 0.680$	$\frac{1}{6}\pi\sqrt{2}$ $= 0.740$

<sup>a</sup>Tables of numbers of neighbors and distances in sc, bcc, fcc, hep, and diamond structures are given on pp. 1037–1039 of J. Hirschfelder, C. F. Curtis and R. B. Bird, *Molecular theory of gases and liquids*, Wiley, 1964.

<sup>b</sup>The packing fraction is the maximum proportion of the available volume that can be filled with hard spheres.

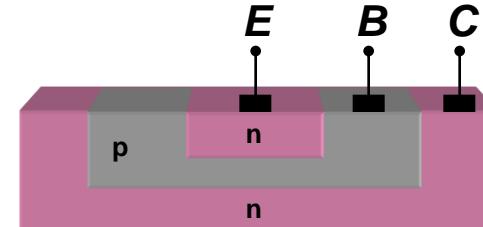
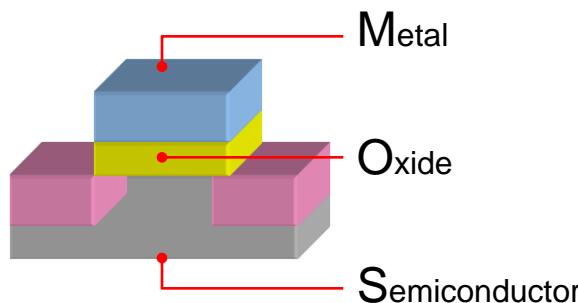
# Crystal structures of Si and GaAs



Diamond & Zincblende (Sphalerite) lattices – **two interpenetrating FCC** sub-lattices one displaced from the other by  $\frac{1}{4}$  of the distance along the diagonal of the cell ( $a\sqrt{3}/4$ )

# Crystallographic planes and directions

- Real crystals are not infinitely large, they terminate at a surface. Semiconductor devices are fabricated near or on the surface, so the surface properties influence the devices' characteristics. Thus, it is very helpful to be able *to determine the planes and directions existent within the lattice.*



# Crystallographic planes and directions

- The orientation of a surface or a crystal plane may be defined by considering how the plane intersects the main crystallographic axes of the solid. The application of a set of rules leads to the assignment of the *Miller Indices*, (*hkl*); a set of numbers which quantify the intercepts and may be used to uniquely identify the plane or surface.

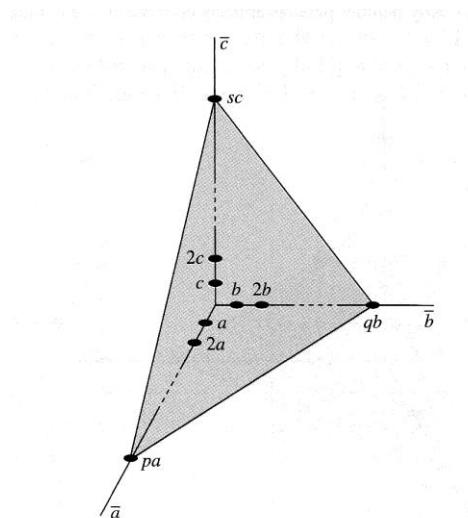


Figure 1.6 | General lattice plane intercepting the  $\bar{a}$ ,  $\bar{b}$ , and  $\bar{c}$  axes at  $p$ ,  $q$ , and  $s$ , respectively.

$$\left( \frac{1}{p}, \frac{1}{q}, \frac{1}{s} \right) \rightarrow (hkl)$$

# Assignment of Miller indices

1. Find the **intercepts of the plane with the crystal axes** and express these intercepts as integral multiples of the basis vectors (the plane can be moved in and out from the origin, retaining its orientation, until such an integral intercept is discovered on each axis).
2. Take the **reciprocals of these three integers** and reduce them to the smallest set of integers ***h*, *k*, and *l***, which have the same relationship to each other as the three reciprocals. Finally, **label the plane (*hkl*)**.

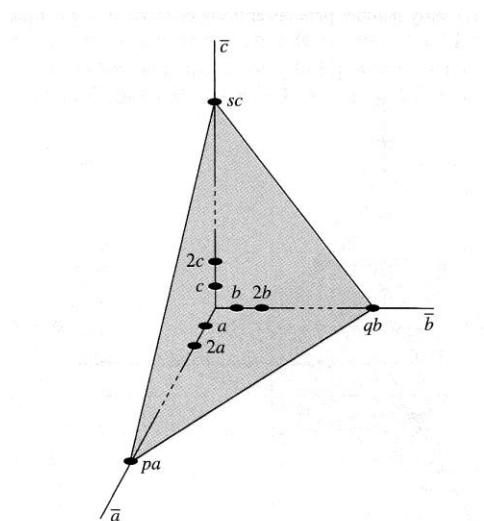


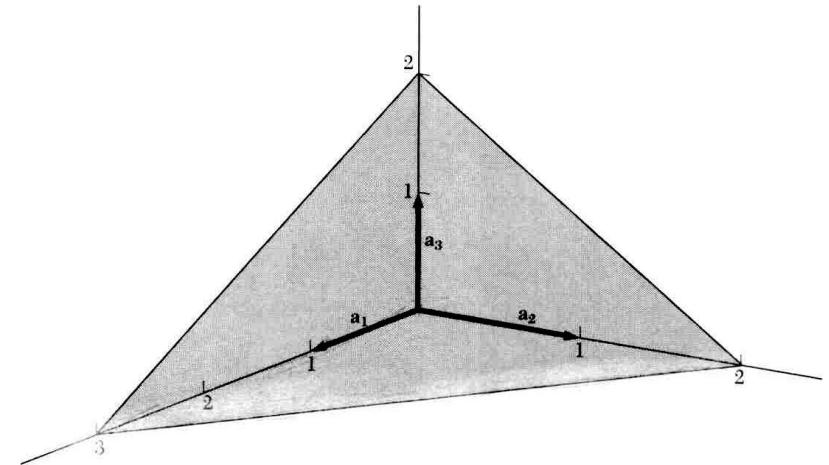
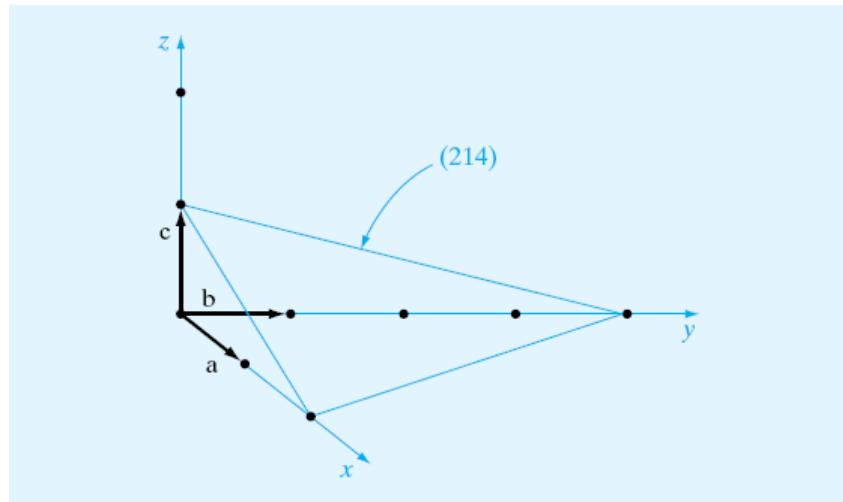
Figure 1.6 | General lattice plane intercepting the  $\bar{a}$ ,  $\bar{b}$ , and  $\bar{c}$  axes at  $p$ ,  $q$ , and  $s$ , respectively.

$$\left( \frac{1}{p}, \frac{1}{q}, \frac{1}{s} \right) \rightarrow (hkl)$$

# Crystallographic planes and directions

$$\left(\frac{1}{2}, \frac{1}{4}, \frac{1}{1}\right) \rightarrow (214)$$

$$\left(\frac{1}{3}, \frac{1}{2}, \frac{1}{2}\right) \rightarrow (233)$$



**Figure 15** This plane intercepts the  $\mathbf{a}_1$ ,  $\mathbf{a}_2$ ,  $\mathbf{a}_3$  axes at  $3\mathbf{a}_1$ ,  $2\mathbf{a}_2$ ,  $2\mathbf{a}_3$ . The reciprocals of these numbers are  $\frac{1}{3}$ ,  $\frac{1}{2}$ ,  $\frac{1}{2}$ . The smallest three integers having the same ratio are 2, 3, 3, and thus the indices of the plane are (233).

# Crystallographic planes and directions

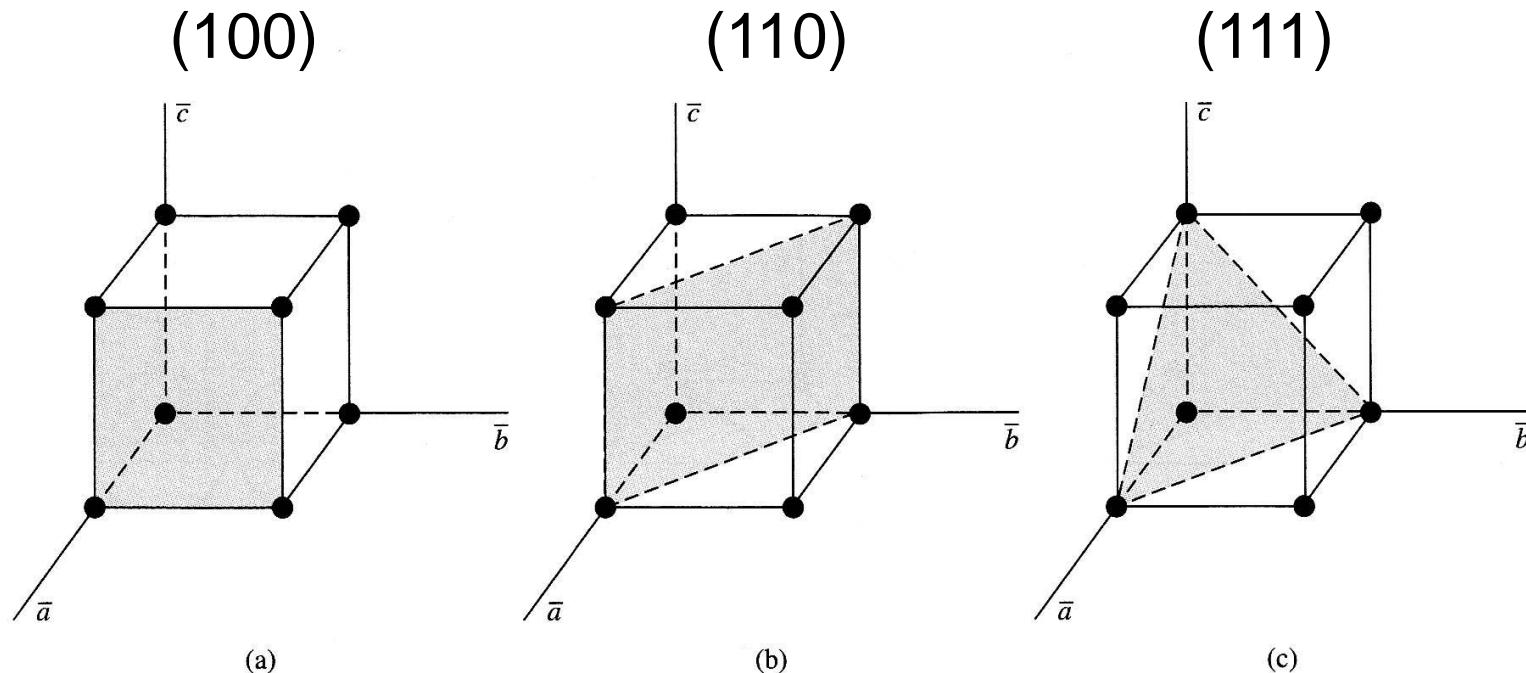


Figure 1.8 | Three lattice planes in a simple cubic lattice: (a) (100) plane, (b) (110) plane, and (c) (111) plane.

Some conventions are given as follows:

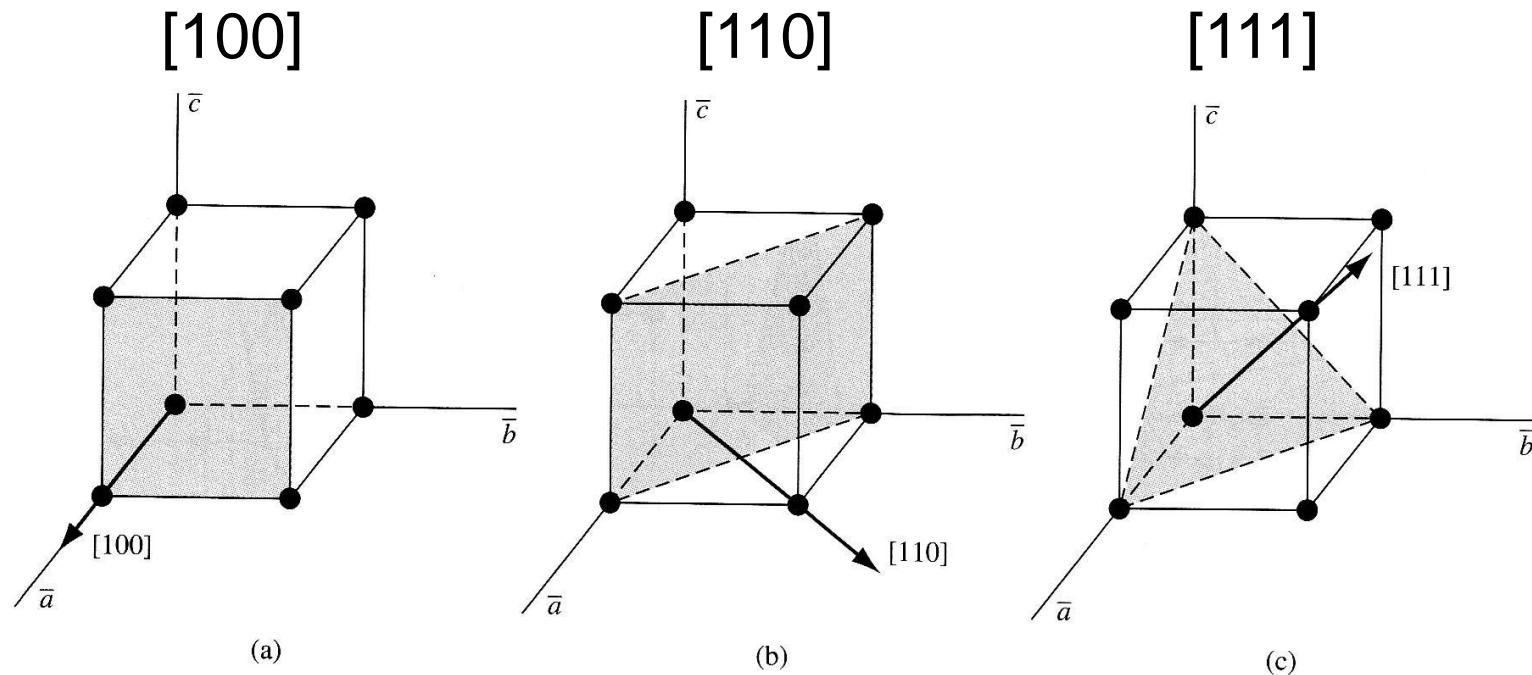
$(h, k, l)$  for a plane

$\{h, k, l\}$  for planes with equivalent symmetry

$[h, k, l]$  for a crystal direction

$\langle h, k, l \rangle$  for a full set of equivalent directions

# Crystallographic planes and directions



**Figure 1.10** | Three lattice planes and directions in a simple cubic lattice: (a) (100) plane and [100] direction, (b) (110) plane and [110] direction, and (c) (111) plane and [111] direction.

Some conventions are given as follows:

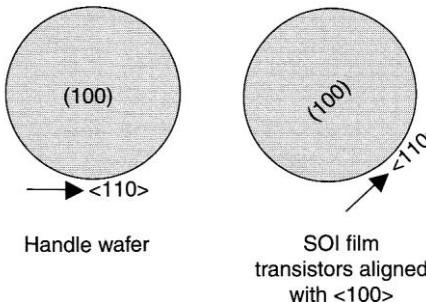
$(h, k, l)$  for a plane

$\{h, k, l\}$  for planes with equivalent symmetry

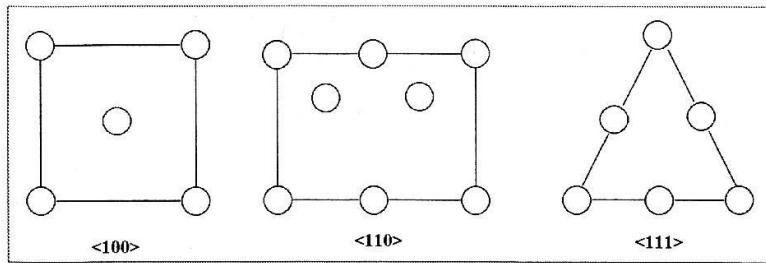
$[h, k, l]$  for a crystal direction

$\langle h, k, l \rangle$  for a full set of equivalent directions

# Crystallographic planes and directions



The concept of a 45-degree rotation of the Si film on insulator.



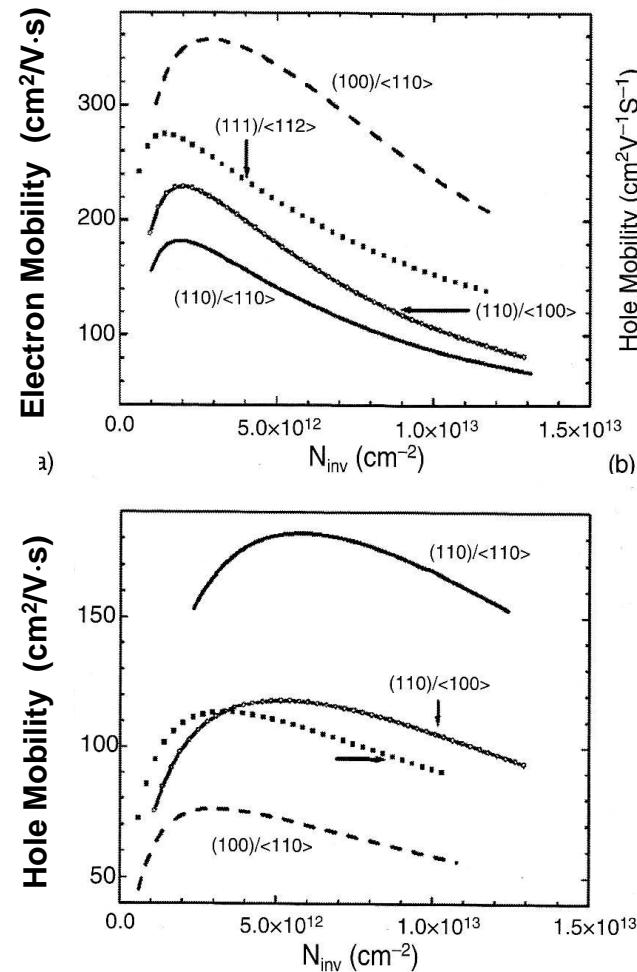
A primera vista se observa un primer indicio del origen del comportamiento anisotrópico del material:

La celda (110) tiene un sitio de adsorción de mayor área que la celda (100).

La celda (111) tiene una malla tan cerrada que prácticamente no presenta sitio de adsorción alguno disponible.

Esto quiere decir, que la probabilidad de adsorción de un ión será mayor para la orientación (110) que para la (100).

La orientación (111) tendrá la probabilidad de adsorción más baja de todas.



Yang M., et al., IEDM (2003).