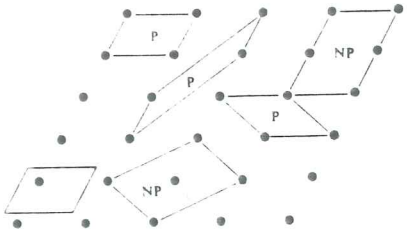
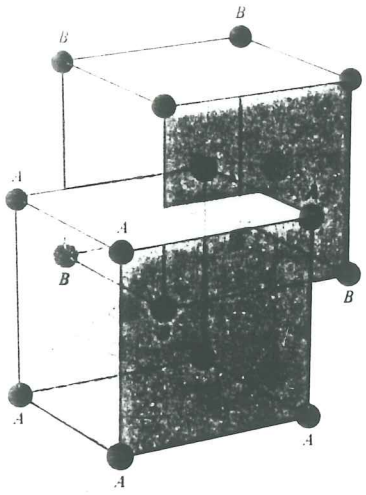
CELLA PRIMITIVA



P = primitive unit cell
NP = nonprimitive unit cell

- SCELTA NON UNICA
- 1 PUNTO RETICOLARE
- RIEMPIE TUTTO LO SPAZIO SENZA SOVRAPPOSIZIONI

Figure 4.5
A few sites from a body-centered cubic Bravais lattice. Note that it can be regarded either as a simple cubic lattice formed from the points A with the points B at the cube centers, or as a simple cubic lattice formed from the points B with the points A at the cube centers. This observation establishes that it is indeed a Bravais lattice.



RETICOLO DI BRAVAIS

↓

COSTRUZIONE GEOMETRICA

$$\mathbf{a}_1 = a\hat{\mathbf{x}}, \quad \mathbf{a}_2 = a\hat{\mathbf{y}}, \quad \mathbf{a}_3 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}}). \tag{4.3}$$

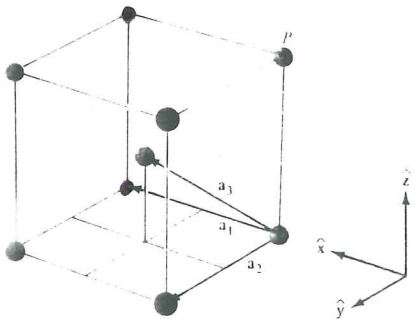


Figure 4.6
Three primitive vectors, specified in Eq. (4.3), for the body-centered cubic Bravais lattice. The lattice is formed by taking all linear combinations of the primitive vectors with integral coefficients. The point P, for example, is $P = -\mathbf{a}_1 - \mathbf{a}_2 + 2\mathbf{a}_3$.

Cr a=2.88 A
Fe a= 2.87 A
Mo a=3.15 A
Ta a= 3.31 A
W a= 3.16A

BCC

DUE POSSIBILI SCELTE DI VETTORI PRIMITIVI

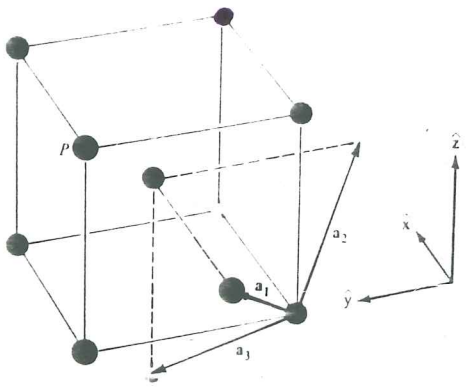


Figure 4.7
A more symmetric set of primitive vectors, specified in Eq. (4.4), for the body-centered cubic Bravais lattice. The point P, for example, has the form $P = 2\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3$.

$\mathbf{a_1}$=a/2(-**x**+**y**+**z**) $\mathbf{a_2}$= a/2(**x**-**y**+**z**) $\mathbf{a_3}$=a/2(**x**-**y**+**z**)

2 punti reticolari per cella convenzionale:
0, a/2(**x**+**y**+**z**)

FCC: Face centered cubic crystal structure

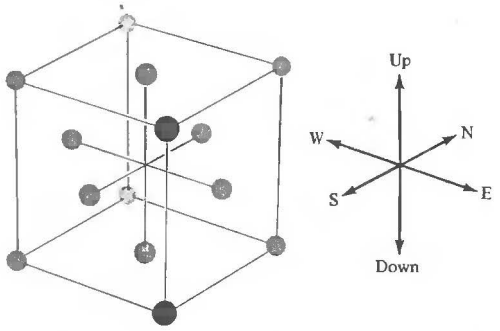


Figure 4.8
Some points from a face-centered cubic Bravais lattice.

A symmetric set of primitive vectors for the face-centered cubic lattice (see Figure 4.9) is

$$\mathbf{a}_1 = \frac{a}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}}), \quad \mathbf{a}_2 = \frac{a}{2}(\hat{\mathbf{z}} + \hat{\mathbf{x}}), \quad \mathbf{a}_3 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}}). \tag{4.5}$$

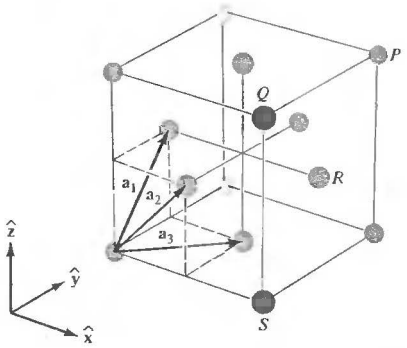


Figure 4.9
A set of primitive vectors, as given in Eq. (4.5), for the face-centered cubic Bravais lattice. The labeled points are $P = \mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3$, $Q = 2\mathbf{a}_2$, $R = \mathbf{a}_2 + \mathbf{a}_3$, and $S = -\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3$.

Ag a= 4.09 A
Al a= 4.05 A
Au a= 4.08 A
Ca a= 5.58 A
Cu a= 3.61 A
Pt a= 3.92 A
....

4 punti reticolari per cella convenzionale:
0, a/2(**x**+**y**), a/2(**y**+**z**), a/2(**x**+**z**)

CELLA PRIMITIVA 3 DIMENSIONI

WIGNER SEITZ

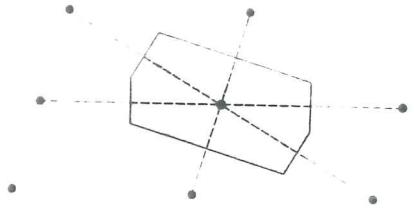
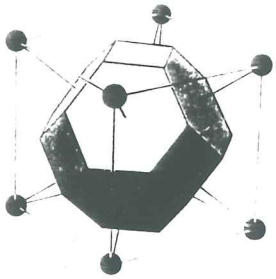


Figure 4.14
The Wigner-Seitz cell for a two-dimensional Bravais lattice. The six sides of the cell bisect the lines joining the central points to its six nearest neighboring points (shown as dashed lines). In two dimensions the Wigner-Seitz cell is always a hexagon unless the lattice is rectangular (see Problem 4a).

Figure 4.15
The Wigner-Seitz cell for the body-centered cubic Bravais lattice (a "truncated octahedron"). The surrounding cube is a conventional body-centered cubic cell with a lattice point at its center and on each vertex. The hexagonal faces bisect the lines joining the central point to the points on the vertices (drawn as solid lines). The square faces bisect the lines joining the central point to the central points in each of the six neighboring cubic cells (not drawn). The hexagons are regular (see Problem 4d).



BCC

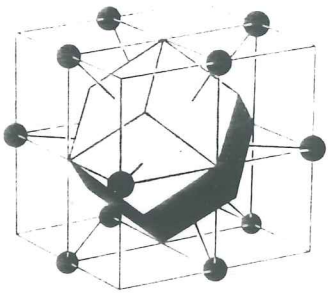


Figure 4.16
Wigner-Seitz cell for the face-centered cubic Bravais lattice (a "rhombic dodecahedron"). The surrounding cube is *not* the conventional cubic cell of Figure 4.12, but one in which lattice points are at the center of the cube and at the center of the 12 edges. Each of the 12 (congruent) faces is perpendicular to a line joining the central point to a point on the center of an edge.

FCC

STRUTTURA CRISTALLINA
=
RETICOLO DI BRAVAIS + BASE

Si → DIAMANTE → F.C.C. + 2 atomi base

GaAs → Zincoblende → F.C.C. + 2 atomi (diversi) base

RETICOLI DI BRAVAIS

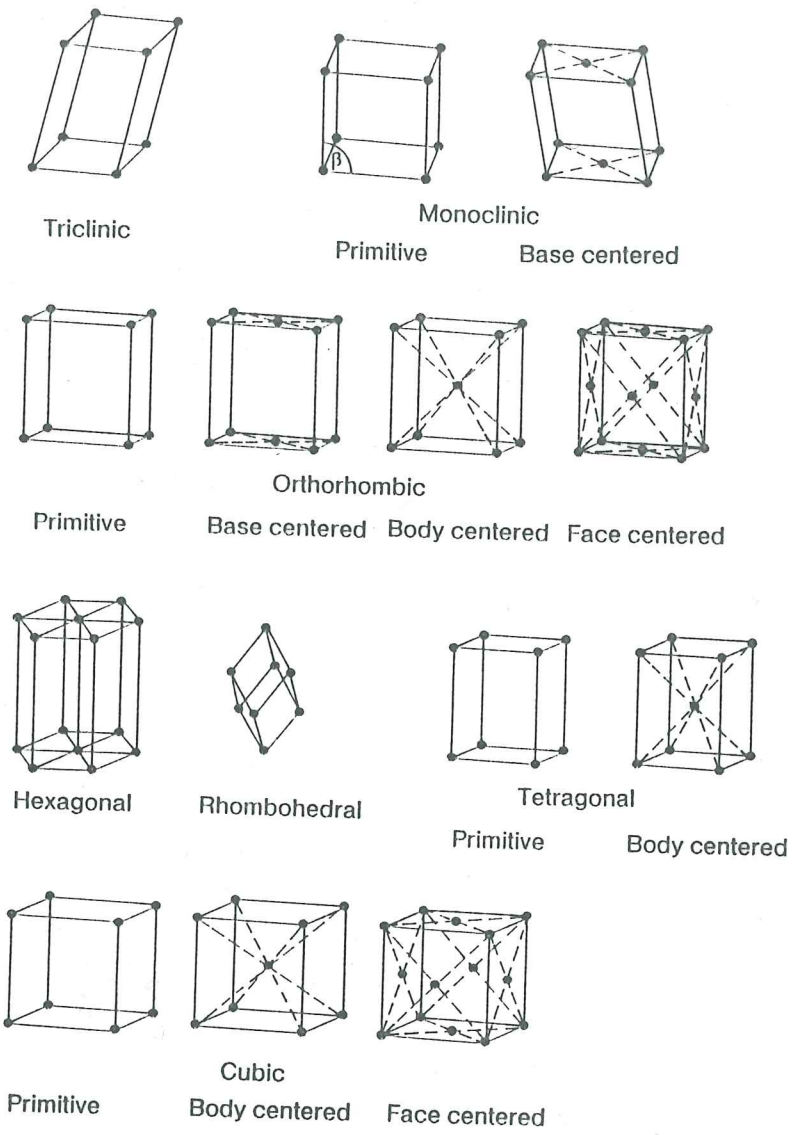


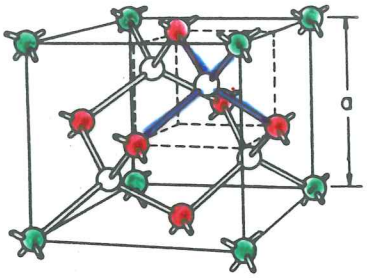
Fig. 2.3. The 14 three-dimensional Bravais lattices. The hexagonal lattice and the two centered cubic lattices are particularly important in solid state physics

Table 2.1. The seven different basis-vector systems or crystal systems. Most elements crystallize in a cubic or hexagonal structure. For this reason, and also because of their high symmetry, the cubic and hexagonal coordinate systems are particularly important

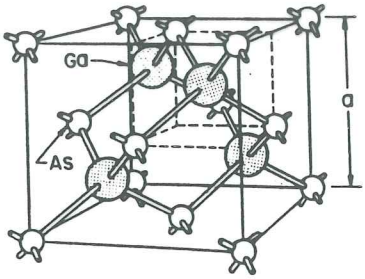
Basis vectors/crystal axes	Angles	Crystal system
$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90°$	triclinic
$a \neq b \neq c$	$\alpha = \gamma = 90° \; \beta \neq 90°$	monoclinic
$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$	orthorhombic
$a = b \neq c$	$\alpha = \beta = \gamma = 90°$	tetragonal
$a = b \neq c$	$\alpha = \beta = 90° \; \gamma = 120°$	hexagonal
$a = b = c$	$\alpha = \beta = \gamma \neq 90°$	rhombohedral
$a = b = c$	$\alpha = \beta = \gamma = 90°$	cubic

STRUTTURA CRISTALLINA

- FACCIA
- vertici
- 1 legame tetraedrico



DIAMOND
(C, Ge, Si, etc)

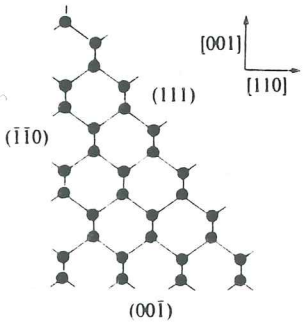


ZINCBLENDE
(GaAs, GaP, etc)

C (diamante) a= 3.57 A
Si a= 5.43 A
Ge a= 5.66 A

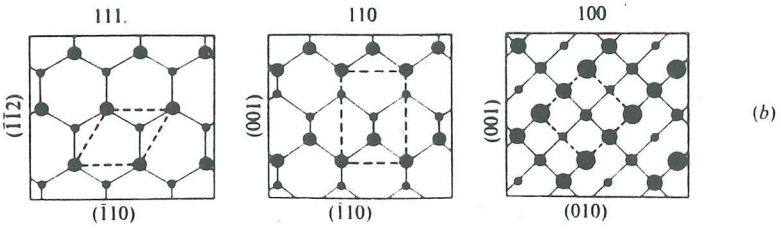
GaAs a= 5.65 A
GaP a= 5.45 A
GaSb a= 6.12 A
InAs a= 6.04 A

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).

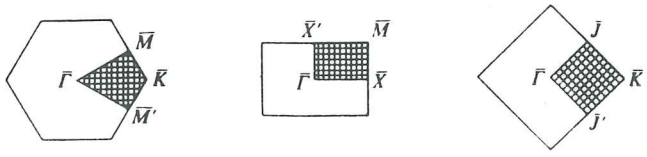


SENZA RICOSTRUZIONE

(*a*)



(*b*)



(*c*)