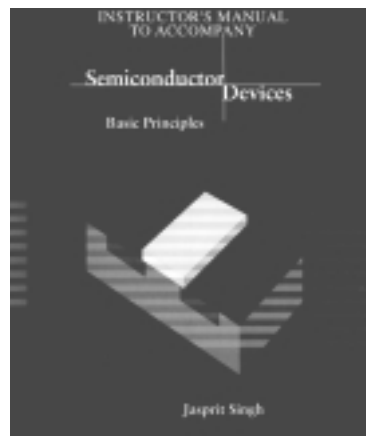

Chapter

1

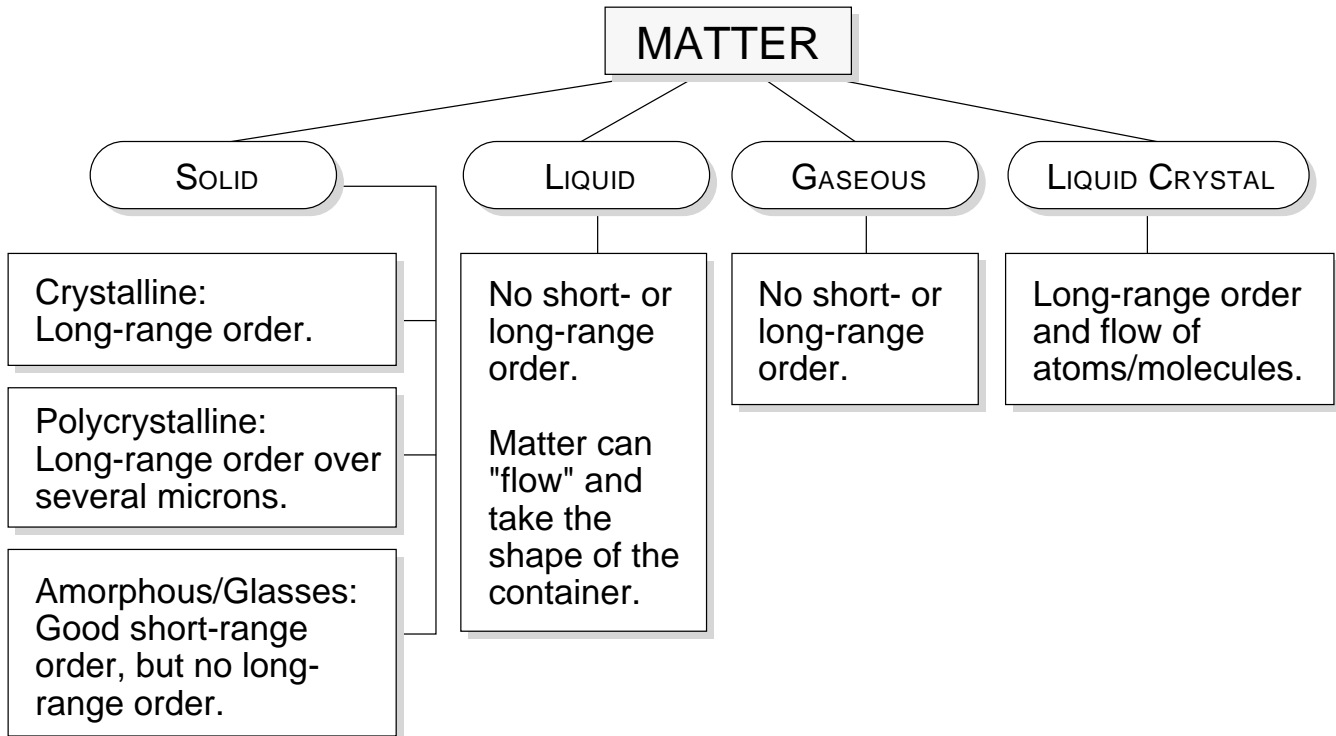
STRUCTURAL ISSUES IN SEMICONDUCTORS



Most semiconductor devices are made from crystalline materials. The following figures provide an overview of important crystalline properties of semiconductors, like Si, GaAs, etc.

SEMICONDUCTORS: STRUCTURAL ISSUES

Different states of matter and a classification based on the order present in the material.



Semiconductors used in most technologies are high quality crystalline materials (some exceptions are amorphous silicon, used for thin film transistor and solar cells).

CRYSTALLINE MATERIALS: SOME DEFINITIONS

BRAVAIS LATTICE: Collection of points that fill up space. Every point has the same environment around it.

TRANSLATION VECTORS: A translation of the crystal by a vector T that takes a point R to $R+T$ and leaves the entire crystal invariant.

PRIMITIVE TRANSLATION VECTORS: Starting at any particular lattice point, we can construct 3 vectors that take us to 3 nearest neighbors points (non-coplanar). The smallest such vectors are called primitive vectors a_1, a_2, a_3 .

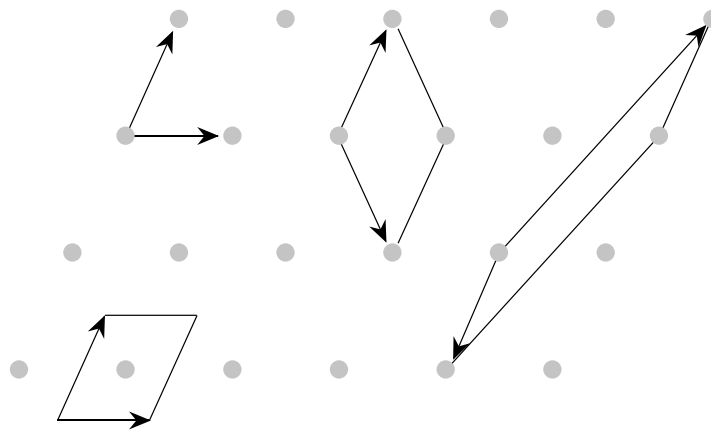
BASIS: A crystal is produced by attaching a basis to every lattice point. The basis consists of one or more atoms.

PRIMITIVE CELL: The primitive vectors define a parallelepiped of volume

$$\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$$

which is called the primitive cell.

There are many different ways of selecting a primitive cell.



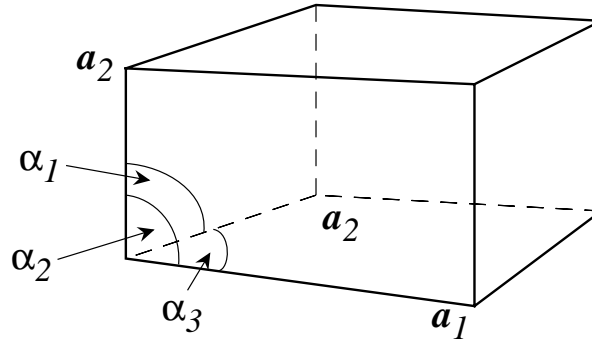
Alternative primitive cell for 2D lattices.

The shape of the primitive cell can be defined by a set of parameters

$$a_1 = |\mathbf{a}_1|; a_2 = |\mathbf{a}_2|; a_3 = |\mathbf{a}_3|$$

$$\alpha_1 = \cos^{-1} \frac{\mathbf{a}_2 \cdot \mathbf{a}_3}{a_2 a_3}; \alpha_2 = \cos^{-1} \frac{\mathbf{a}_1 \cdot \mathbf{a}_3}{a_1 a_3}; \alpha_3 = \cos^{-1} \frac{\mathbf{a}_1 \cdot \mathbf{a}_2}{a_1 a_2}$$

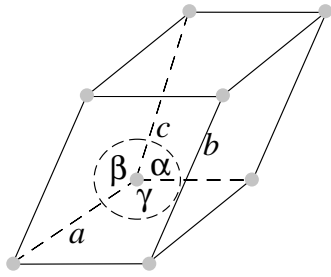
Notation for a primitive cell.



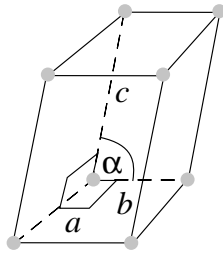
Bravais lattices can be formed only if

$$\alpha = 0; \frac{\pi}{3} \text{ or } \frac{5\pi}{3}; \frac{\pi}{2} \text{ or } \frac{3\pi}{2}; \frac{2\pi}{3} \text{ or } \frac{4\pi}{3}; \pi$$

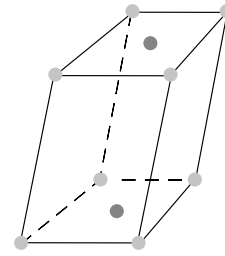
System	Number of lattices	Restrictions on conventional cell axes and angles
Triclinic	1	$a_1 \neq a_2 \neq a_3$ $\alpha \neq \beta \neq \gamma$
Monoclinic	2	$a_1 \neq a_2 \neq a_3$ $\alpha = \gamma = 90^\circ \neq \beta$
Orthorhombic	4	$a_1 \neq a_2 \neq a_3$ $\alpha = \beta = \gamma = 90^\circ$
Tetragonal	2	$a_1 = a_2 \neq a_3$ $\alpha = \beta = \gamma = 90^\circ$
Cubic	3	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90^\circ$
Trigonal	1	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma < 120^\circ, \neq 90^\circ$
Hexagonal	1	$a_1 = a_2 \neq a_3$ $\alpha = \beta = 90^\circ \neq \gamma$ $\gamma = 120^\circ$



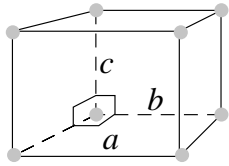
triclinic



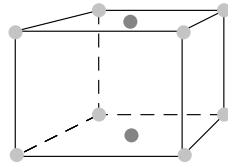
monoclinic



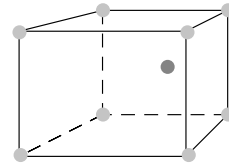
base-centered



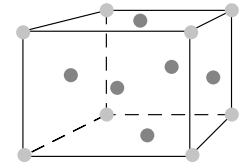
orthorhombic



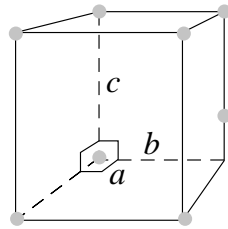
base-centered



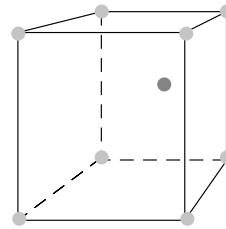
body-centered



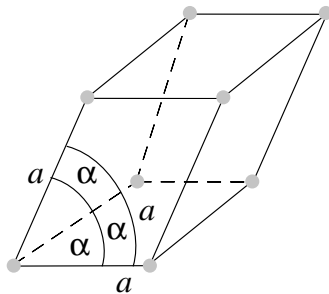
face-centered



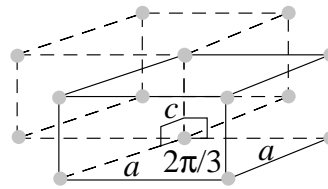
tetragonal



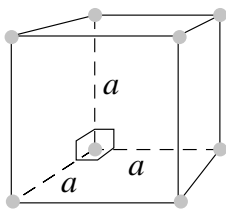
body-centered



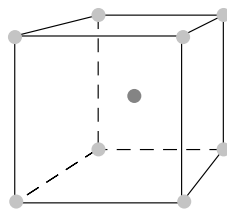
rhombohedral



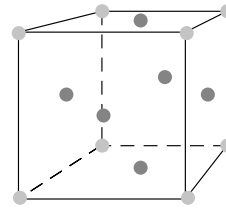
hexagonal



cubic



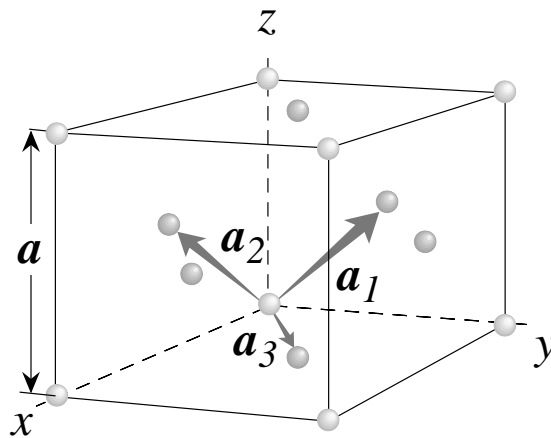
body-cubic



face-centered cubic

Most semiconductors have an underlying lattice that is either face-centered cubic (fcc) or hexagonal closed pack (hcp).

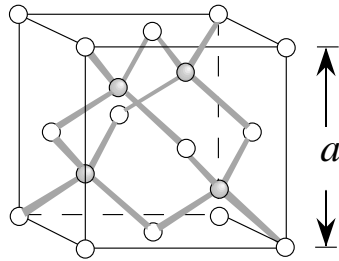
FACE CENTERED CUBIC: The lattice sites at the edges of a cube and at the center of its faces. The edge of the cube a is called the lattice constant.



Primitive basis vectors for the face-centered cubic lattice.

$$\mathbf{a}_1 = \frac{a}{2} (\mathbf{y} + \mathbf{z}), \mathbf{a}_2 = \frac{a}{2} (\mathbf{z} + \mathbf{x}), \mathbf{a}_3 = \frac{a}{2} (\mathbf{x} + \mathbf{y})$$

DIAMOND AND ZINC BLENDE STRUCTURES



The zinc blende crystal structure. The structure consists of the interpenetrating fcc lattices, one displaced from the other by a distance $\left(\frac{a}{4}, \frac{a}{4}, \frac{a}{4}\right)$ along the body diagonal. The underlying Bravais lattice is fcc with a two-atom basis. The positions of the two atoms is (000) and $\left(\frac{a}{4}, \frac{a}{4}, \frac{a}{4}\right)$.

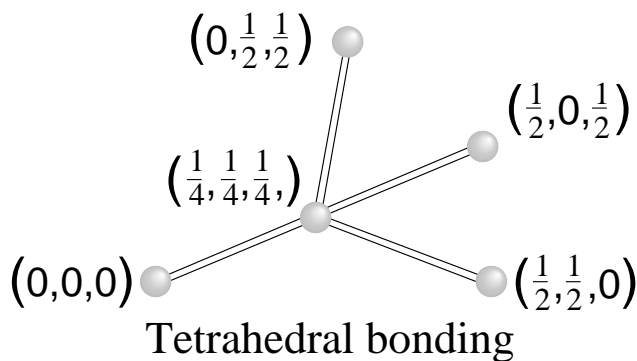
Positions of the atoms

$$\mathbf{A} = (n_1, n_2, n_3), (n_1 + \frac{1}{4}, n_2 + \frac{1}{4}, n_3 + \frac{1}{4}),$$

$$(n_1 + \frac{1}{2}, n_2 + \frac{1}{2}, n_3), (n_1 + \frac{3}{4}, n_2 + \frac{3}{4}, n_3 + \frac{1}{4}),$$

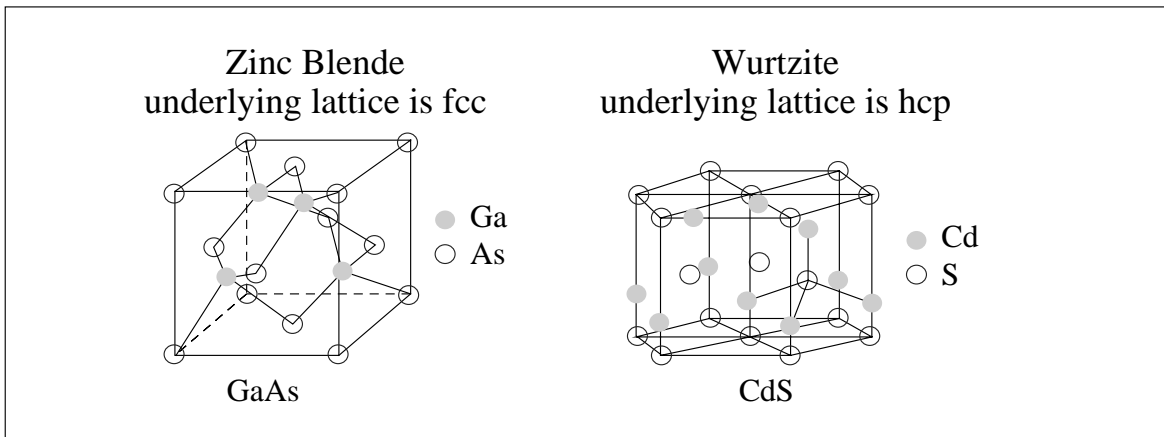
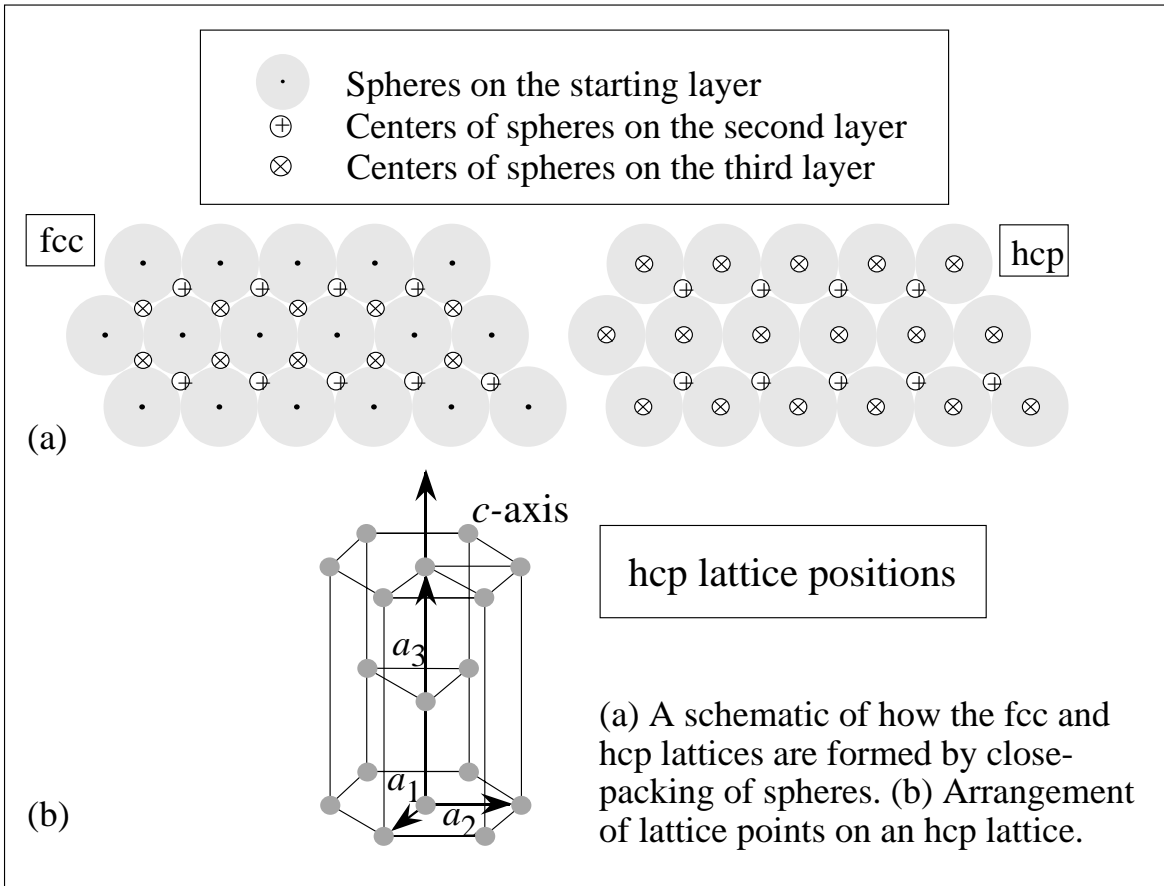
$$(n_1 + \frac{1}{2}, n_2, n_3 + \frac{1}{2}), (n_1 + \frac{3}{4}, n_2 + \frac{1}{4}, n_3 + \frac{3}{4}),$$

$$(n_1, n_2 + \frac{1}{2}, n_3 + \frac{1}{2}), (n_1 + \frac{1}{4}, n_2 + \frac{3}{4}, n_3 + \frac{3}{4})$$

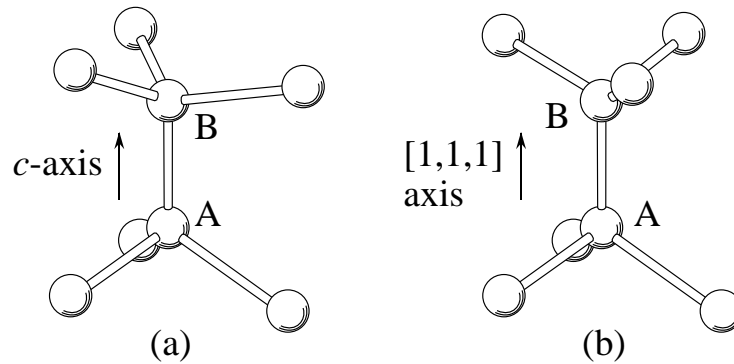


Nature of
chemical bonds
in a diamond
or zinc blende
structure

FCC AND HCP STRUCTURES



ZINC BLENDE AND WURTZITE



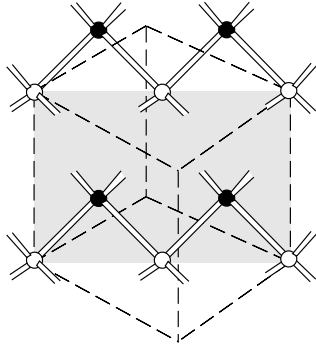
Orientations of adjacent atomic tetrahedra in wurtzite (a) and zinc blende (b). The A and B refer to the two different species of atom.

SEMICONDUCTORS

Elements commonly found in semiconductor compounds

I	II	III	IV	V	VI	VII
	Be	B	C	N	O	F
	Mg	Al	Si	P	S	Cl
Cu	Zn	Ga	Ge	As	Se	Br
Ag	Cd	In	Sn	Sb	Te	I
	Hg	Tl	Pb	Bi		

IMPORTANT PLANES IN ZINC BLENDE OR DIAMOND STRUCTURES

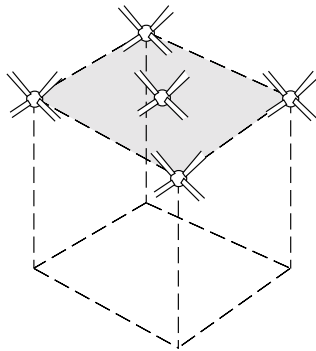


ATOMS ON THE (110) PLANE

Each atom has 4 bonds:

- 2 bonds in the (110) plane
- 1 bond connects each atom to adjacent (110) planes

⇒ Cleaving adjacent planes requires breaking 1 bond per atom.

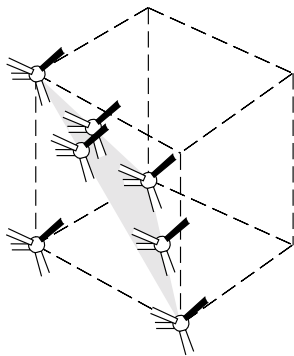


ATOMS ON THE (001) PLANE

2 bonds connect each atom to adjacent (001) plane.

Atoms are either Ga or As in a GaAs crystal.

⇒ Cleaving adjacent planes requires breaking 2 bonds per atom.



ATOMS ON THE (111) PLANE

Could be either Ga or As.

1 bond connecting an adjacent plane on one side.

3 bonds connecting an adjacent plane on the other side.

Some important planes in the cubic system with their Miller indices. This figure also shows how many bonds connect adjacent planes. This number determines how easy or difficult it is to cleave the crystal along these planes by cutting the bonds joining the adjacent planes.