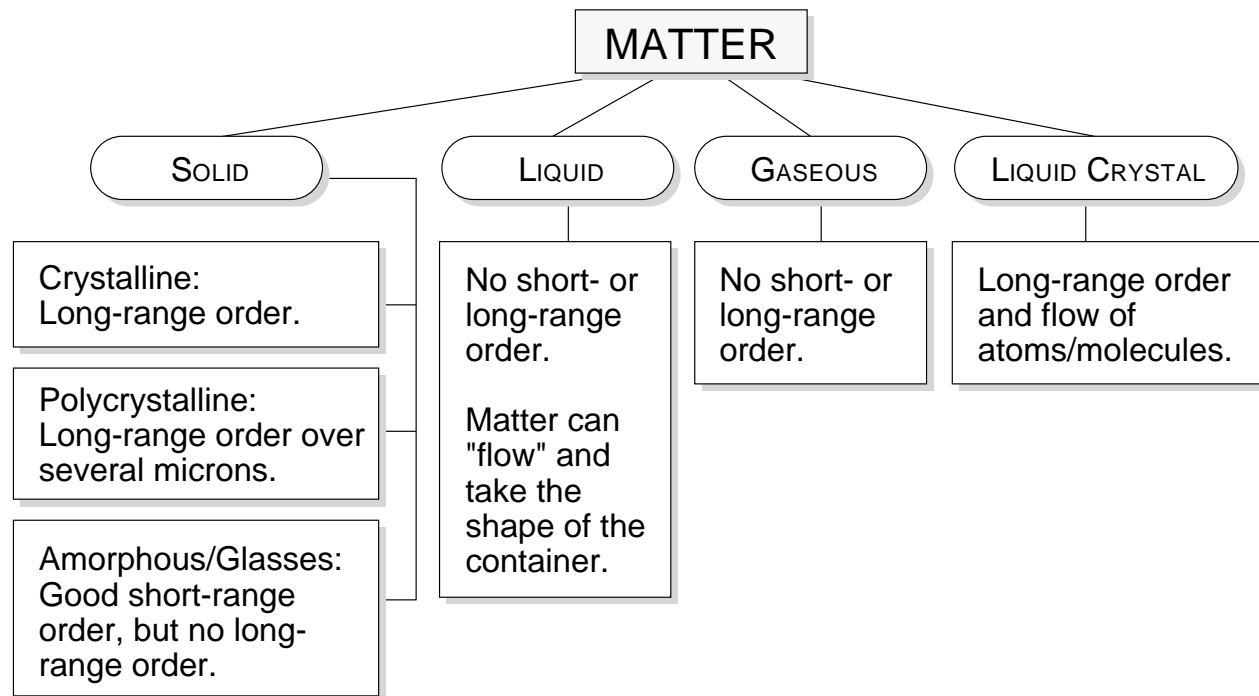

Chapter

1

STRUCTURAL PROPERTIES OF SEMICONDUCTORS

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 .

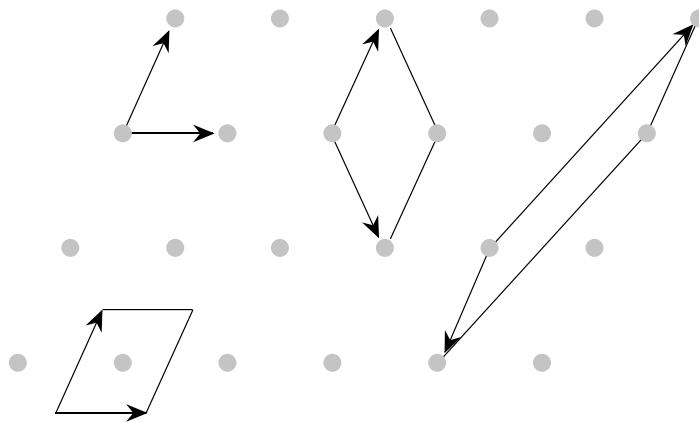
BASIS: A crystal is produced by attaching a basis to every lattice point. The basis consists of one or more atoms.

PRIMITIVE CELL: The primitive vectors define a parallelepiped of volume

$$\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3$$

which is called the primitive cell.

There are many different ways of selecting a primitive cell.



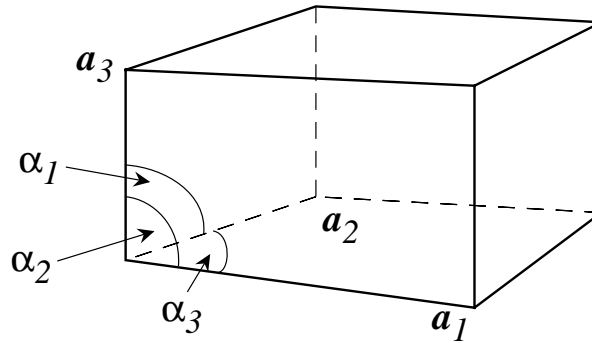
Alternative primitive cell for 2D lattices.

The shape of primitive cells can be defined by a set of parameters

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

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

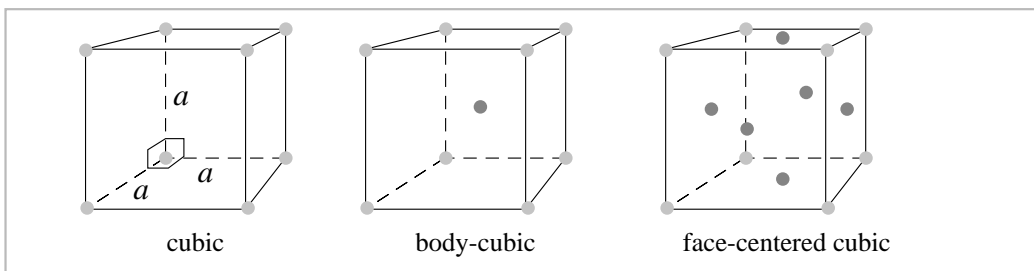
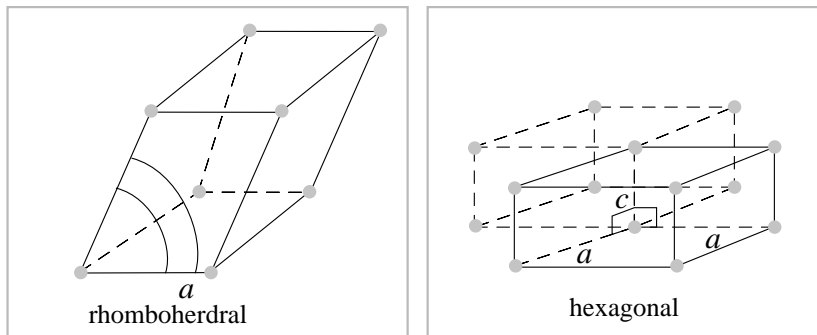
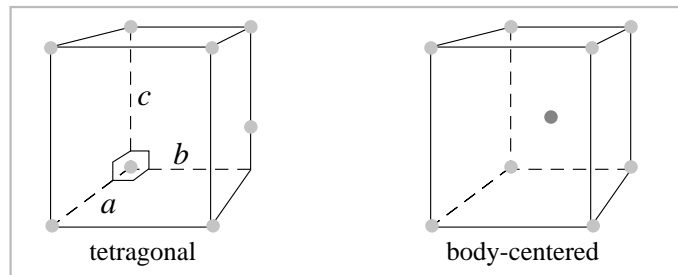
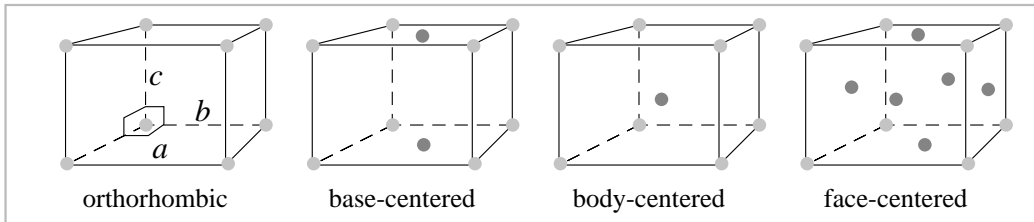
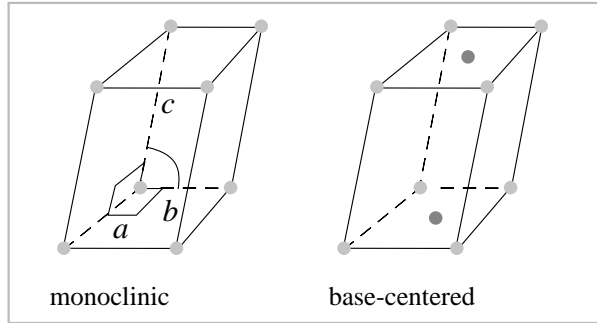
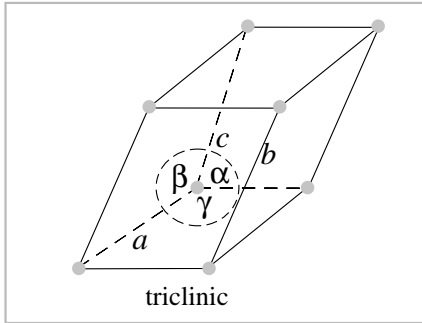
Notation for a primitive cell.



Bravais lattices can be formed only if

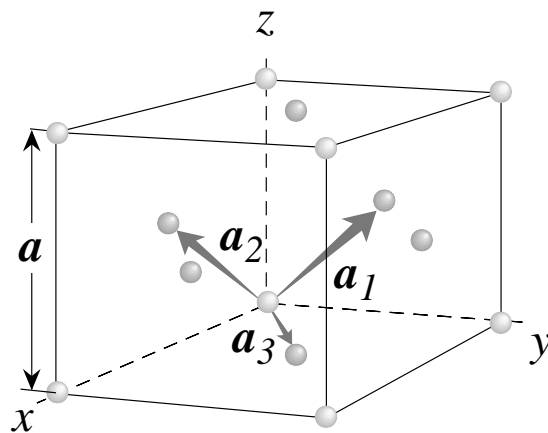
$$\alpha = 0; \frac{\pi}{3} \text{ or } \frac{5\pi}{3}; \frac{\pi}{2} \text{ or } \frac{3\pi}{2}; \frac{2\pi}{3} \text{ or } \frac{4\pi}{3}; \pi$$

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	$a_1 = a_2 \neq a_3$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$



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

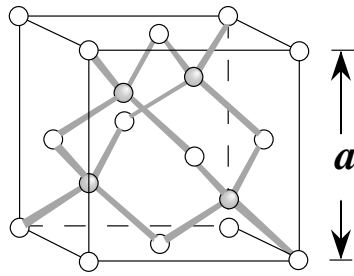
FACE CENTERED CUBIC: The lattice sites at the edges of a cube and at the center of its faces. The edge of the cube a is called the lattice constant.



Primitive basis vectors for the face-centered cubic lattice.

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

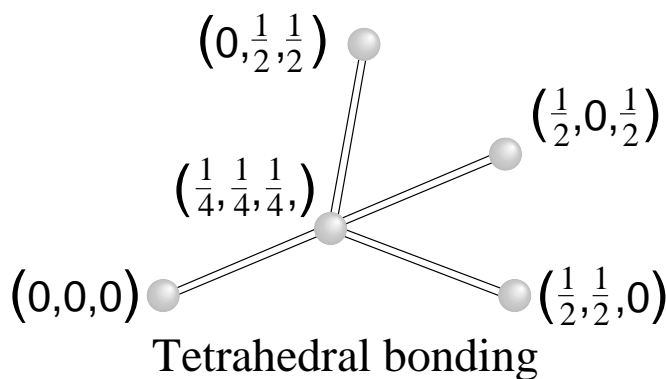
DIAMOND AND ZINC BLENDE STRUCTURES



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

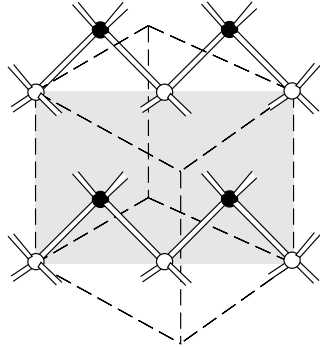
Positions of the atoms

$$\begin{aligned} \mathbf{A} = & (n_1, n_2, n_3), (n_1 + \frac{1}{4}, n_2 + \frac{1}{4}, n_3 + \frac{1}{4}), \\ & (n_1 + \frac{1}{2}, n_2 + \frac{1}{2}, n_3), (n_1 + \frac{3}{4}, n_2 + \frac{3}{4}, n_3 + \frac{1}{4}), \\ & (n_1 + \frac{1}{2}, n_2, n_3 + \frac{1}{2}), (n_1 + \frac{3}{4}, n_2 + \frac{1}{4}, n_3 + \frac{3}{4}), \\ & (n_1, n_2 + \frac{1}{2}, n_3 + \frac{1}{2}), (n_1 + \frac{1}{4}, n_2 + \frac{3}{4}, n_3 + \frac{3}{4}) \end{aligned}$$



Nature of
chemical bonds
in a diamond
or zinc blende
structure

IMPORTANT PLANES IN ZINC BLENDE OR DIAMOND STRUCTURES

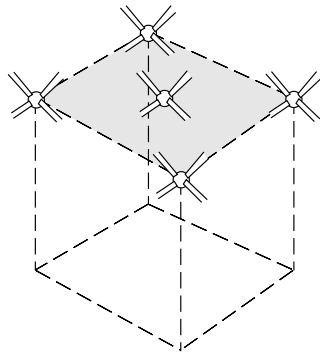


ATOMS ON THE (110) PLANE

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.

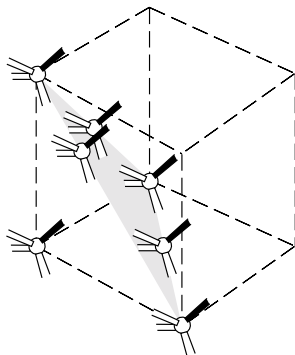


ATOMS ON THE (001) PLANE

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

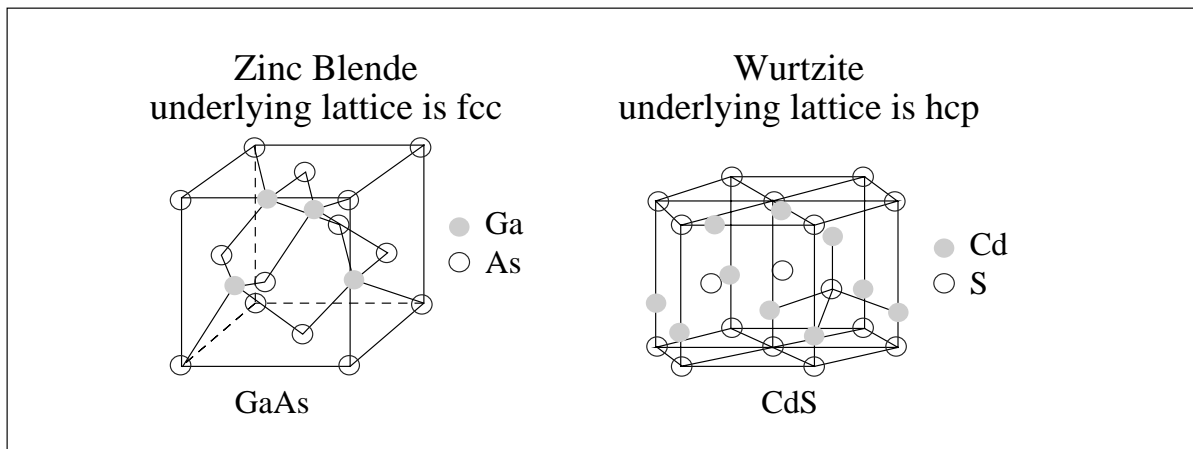
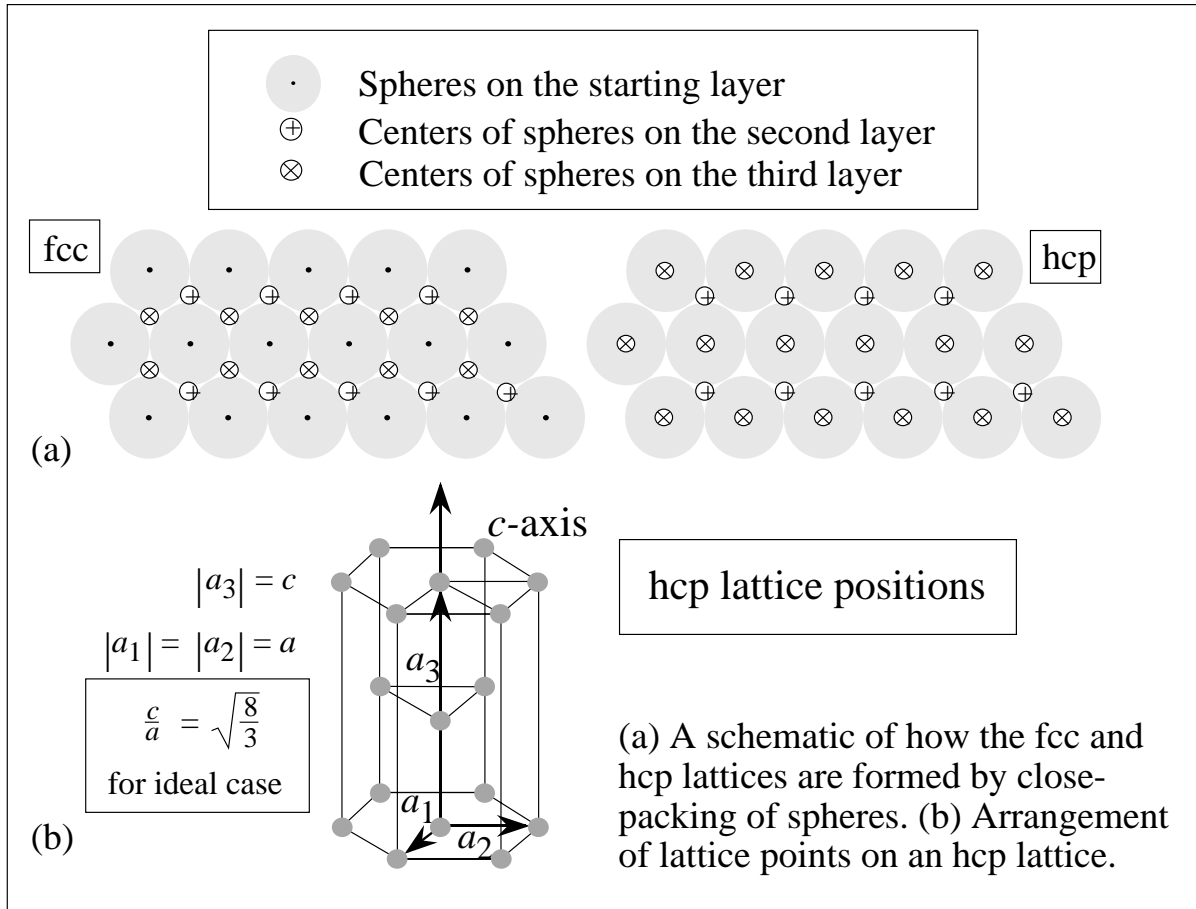
Could be either Ga or As.

1 bond connecting an adjacent plane on one side.

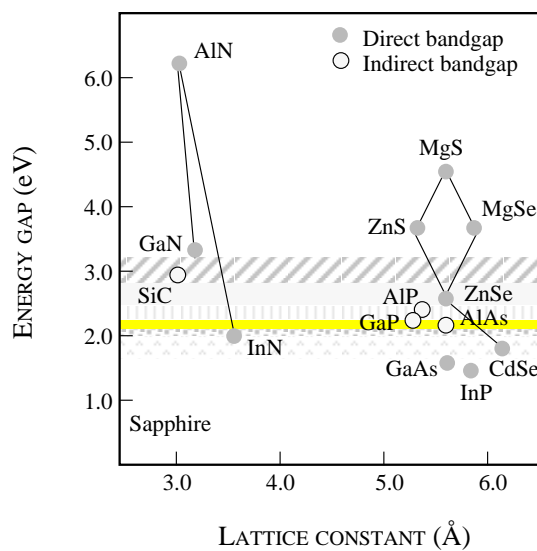
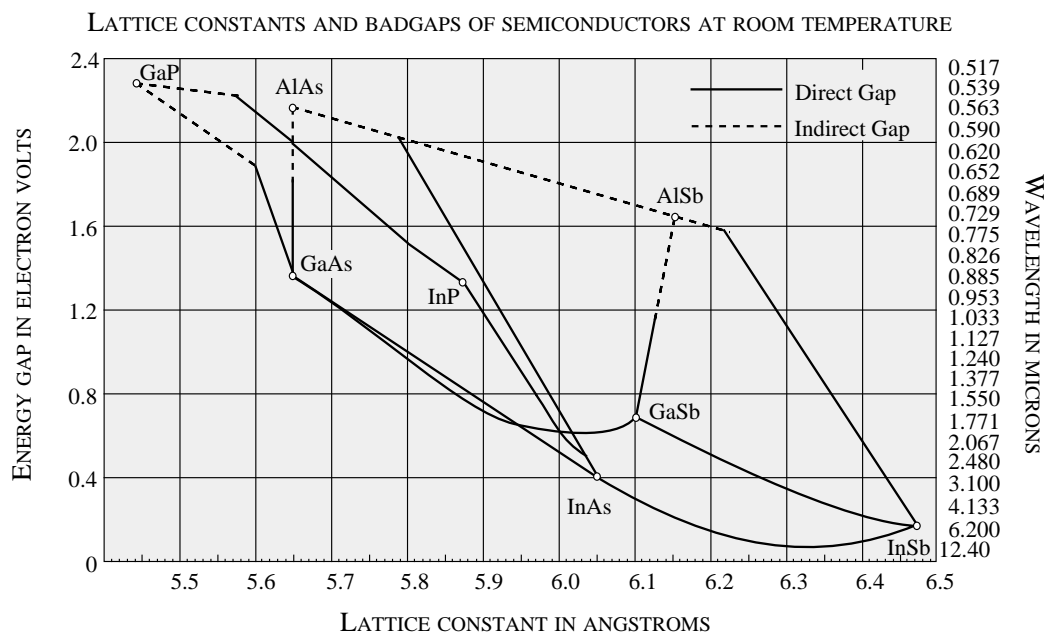
3 bonds connecting an adjacent plane on the other side.

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.

FCC and HCP STRUCTURES



ALLOYS: BANDGAPS AND LATTICE CONSTANTS



IMPORTANT SEMICONDUCTORS: ELECTRONICS

High speed \Rightarrow low effective mass, superior mobility.

High power applications \Rightarrow large bandgap.

High temperature applications \Rightarrow large bandgap.

ADVANTAGES		DISADVANTAGES
Silicon (Si):	The most important semiconductor system. MOSFETs, bipolar devices based on Si form over 90% of the electronic market.	Not as “fast” as other semiconductors. Not good for high power, high temperature operation. Cannot emit light, since it is an indirect gap material.
Silicon-Germanium (Si-Ge):	Can be grown on Si substrates and processed using Si technology. Bipolar devices have performance rivaling GaAs technology.	Strained system. Needs great care in crystal growth conditions.
GaAs; GaAs/AlGaAs:	High speed devices for digital/microwave applications. Performance is superior to silicon.	More expensive than Si technology.
InP; InGaAs/InP:	High speed performance is superior to GaAs based technology. Can be combined with longhaul optoelectronic communication technology.	Expensive.
GaN/AlGaN	High power/high temperature applications.	Not as reliable yet; high cost.
SiC:	High power/high temperature applications.	Reliability; cost.

IMPORTANT SEMICONDUCTORS: OPTOELECTRONICS

Cosiderations:

- Correct bandgap (E_g) for light emission/detection at appropriate wavelength.
- Substrate availability for high quality growth.

LIGHT SOURCES

IMPORTANT MATERIAL SYSTEMS	COMMENTS
$\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$; $x = 0.47y$ for lattice match to InP $E_g = 1.35 - 0.72y + 0.12y^2$ eV	<ul style="list-style-type: none"> • Lattice matched to InP. • Wide range of emission energies can be accessed (~ 0.8 to 1.35 eV). • Material technology is quite advanced and can be exploited for communication applications.
AlGaAs $E_g = 1.43 + 1.25x$ eV; $x \leq 0.35$	<ul style="list-style-type: none"> • Lattice matched to GaAs. • Technology is quite advanced and can be used for LANs.
$\text{GaAs}_{1-x}\text{P}_x$	<ul style="list-style-type: none"> • Material becomes indirect at $x = 0.45$. • With N doping the LED can operate even if the material is indirect and green light emission ($\lambda = 0.55 \mu\text{m}$) can be achieved. • The versatile material can provide red ($\text{GaAs}_{0.6}\text{P}_{0.4}$); orange ($\text{GaAs}_{0.35}\text{P}_{0.65}\text{:N}$), and yellow ($\text{GaAs}_{0.15}\text{P}_{0.85}\text{:N}$) as well.
SiC, GaN, ZnS, ZnSe, AlInGaP —large gap materials which can emit blue light and beyond.	<ul style="list-style-type: none"> • Important materials for blue light emission (for displays, memories). • Technology for optical sources is not mature, but rapid progress is being made.

IMPORTANT SEMICONDUCTORS: OPTOELECTRONICS

DETECTORS

InGaAs (Tunable E_g)	<ul style="list-style-type: none">• Excellent material for long haul communications (at 1.55 μm).• Can be lattice matched to InP.
AlGaSb (Tunable E_g)	<ul style="list-style-type: none">• Excellent optical properties.• Can be used for long haul communications.• Suffers from poor substrate availability, since it has to be grown on GaSb, whose technology is not matured.
InGaAsP (Tunable E_g)	<ul style="list-style-type: none">• Suitable for both 1.55 μm and 1.3 μm applications for long haul applications.• Can be lattice matched to InP substrates.
HgCdTe (Tunable E_g)	<ul style="list-style-type: none">• Excellent material for long wavelength applications in night vision and thermal imaging.• Can be used for 1.55 μm and 1.3 μm, but the technology is not as advanced as the InP based technology.
Si ($E_g = 1.1 \text{ eV}$)	<ul style="list-style-type: none">• Indirect material with small α near the bandedge.• Has high β_{imp}/α_{imp} ratio and can be used in high performance avalanche photodiodes for local area network (LAN) applications.• Not suitable for long haul communication at $\lambda = 1.55 \mu\text{m}$ or 1.3 μm.
Ge ($E_g = 0.7 \text{ eV}$)	<ul style="list-style-type: none">• Indirect material with small α near the bandedge.• Has high β_{imp}/α_{imp} ratio and can be used for avalanche photodiodes for both local area and long distance communications.
GaAs ($E_g = 1.43 \text{ eV}$)	<ul style="list-style-type: none">• Direct gap material.• Not suitable for high quality avalanche detectors, since $\alpha_{imp} \approx \beta_{imp}$.• Not suited for long distance or LAN applications.

Zinc Blende and Wurtzite

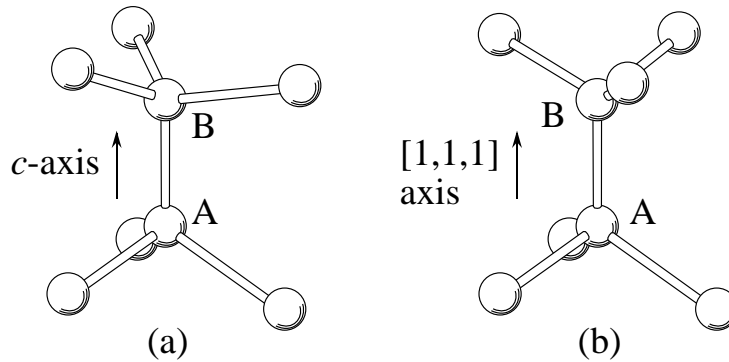
MATERIAL	CRYSTAL STRUCTURE	BANDGAP (eV)	STATIC DIELECTRIC CONSTANT	LATTICE CONSTANT (Å)	DENSITY (gm-cm ⁻³)
C	DI	5.50, I	5.570	3.56683	3.51525
Si	DI	1.1242, I	11.9	5.431073	2.329002
SiC	ZB	2.416, I	9.72	4.3596	3.166
Ge	DI	0.664, I	16.2	5.6579060	5.3234
BN	HEX	5.2, I	$\epsilon_{ } = 5.06$ $\epsilon_{\perp} = 6.85$	$a = 6.6612$ $c = 2.5040$	2.18
BN	ZB	6.4, I	7.1	3.6157	3.4870
BP	ZB	2.4, I	11.	4.5383	2.97
BAs	ZB	—	—	4.777	5.22
AlN	W	6.2, D	$\bar{\epsilon} = 9.14$	$a = 3.111$ $c = 4.981$	3.255
AlP	ZB	2.45, I	9.8	5.4635	2.401
AlAs	ZB	2.153, I	10.06	5.660	3.760
AlSb	ZB	1.615, I	12.04	6.1355	4.26
GaN	W	3.44, D	$\epsilon_{ } = 10.4$ $\epsilon_{\perp} = 9.5$	$a = 3.175$ $c = 5.158$	6.095
GaP	ZB	2.272, I	11.11	5.4505	4.138
GaAs	ZB	1.4241, D	13.18	5.65325	5.3176
GaSb	ZB	0.75, D	15.69	6.09593	5.6137
InN	W	1.89, D	—	$a = 3.5446$ $c = 8.7034$	6.81
InP	ZB	1.344, D	12.56	5.8687	4.81
InAs	ZB	0.354, D	15.15	6.0583	5.667
InSb	ZB	0.230, D	16.8	6.47937	5.7747
ZnO	W	3.44, D	$\epsilon_{ } = 8.75$ $\epsilon_{\perp} = 7.8$	$a = 3.253$ $c = 5.213$	5.67526
ZnS	ZB	3.68, D	8.9	5.4102	4.079
ZnS	W	3.9107, D	$\bar{\epsilon} = 9.6$	$a = 3.8226$ $c = 6.2605$	4.084
ZnSe	ZB	2.8215, D	9.1	5.6676	5.266
ZnTe	ZB	2.3941, D	8.7	6.1037	5.636
CdO	R	0.84, I	21.9	4.689	8.15
CdS	W	2.501, D	$\bar{\epsilon} = 9.83$	$a = 4.1362$ $c = 6.714$	4.82
CdS	ZB	2.50, D	—	5.818	—
CdSe	W	1.751, D	$\epsilon_{ } = 10.16$ $\epsilon_{\perp} = 9.29$	$a = 4.2999$ $c = 7.0109$	5.81
CdSe	ZB	—	—	6.052	—
CdTe	ZB	1.475, D	10.2	6.482	5.87
PbS	R	0.41, D*	169.	5.936	7.597
PbSe	R	0.278, D*	210.	6.117	8.26
PbTe	R	0.310, D*	414.	6.462	8.219

Data are given at room temperature values (300 K).

Key: DI: diamond; HEX: hexagonal; R: rocksalt; W: wurtzite; ZB: zinc blende;

*: gap at L point; D: direct; I: indirect $\epsilon_{||}$: parallel to c -axis; ϵ_{\perp} : perpendicular to c -axis

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		

Bandgaps (in eV) of some semiconductors

TETRAHEDRALLY BONDED MATERIALS					i: Indirect gap D: Diamond Z: Zinc Blende W: Wurtzite R: Rocksalt O: Orthorhombic Rh: Rhombohedral T: Trigonal OR: Orthorhombic distorted rocksalt M: Monoclinic
V	C	Si	Ge	α -Sn	
C	5.5i,D				
Si	2.6i,Z/W	1.1i,D	0.7-1.1i		
Ge		0.7-1.1	0.74i,D		
α -Sn				0.09,D	
III-V	N	P	As	Sb	
B	3.8,W	2.0i,Z	1.5i,Z		
Al	5.9,W	2.5,Z	2.2,Z	1.7,Z	
Ga	3.5,W	2.4i,Z	1.5,Z	0.81,Z	
In	0.9,W	1.4,Z	0.41,Z	0.24,Z	
II-VI	O	S	Se	Te	
Zn	3.4,W	3.6,Z/W	2.8,Z/W	2.4,Z	i: Indirect gap D: Diamond Z: Zinc Blende W: Wurtzite R: Rocksalt O: Orthorhombic Rh: Rhombohedral T: Trigonal OR: Orthorhombic distorted rocksalt M: Monoclinic
Cd	1.3i,R	2.5,Z/W	1.8,Z/W	1.6,Z	
Hg	2.2,O/Rh	2.3,T	-.06,Z	-.3,Z	
I-VII	F	Cl	Br	I	
Cu		3.4,Z	3.1,Z	3.1,Z	
Ag	2.8i,R	3.2i,R	2.7i,R	3.0,W	

NON-TETRAHEDRAL BONDED MATERIALS

IV-VI compounds

IV-VI	O	S	Se	Te
Ge		1.7,OR	1.1,OR	0.15,R
Sn		1.1,OR	0.9,OR	2.1,R
Pb	2.0,i	0.29,R	0.15,R	0.19,R

Group VI elements

VI	S	Se	Te
	3.6,O	1.9i,T 2.5,M	0.33,T

Group V elements

V	P	As	Sb	Bi
	.33,O	.17,Rh	.10	.015