# 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).

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## **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 parallelopiped of volume $a_1 \cdot a_2 \times a_3$

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

$$a_1 = |a_1|; a_2 = |a_2|; a_3 = |a_3|$$

$$\alpha_1 = \cos^{-1} \frac{a_2 \cdot a_3}{a_2 a_3}; \ \alpha_2 = \cos^{-1} \frac{a_1 \cdot a_3}{a_1 a_3}; \ \alpha_3 = \cos^{-1} \frac{a_1 \cdot a_2}{a_1 a_2}$$

Notation for a primitive cell.



Bravais lattices can be formed only if

$\alpha = 0; \ \frac{\pi}{3}$ or	$\frac{5\pi}{3};\frac{\pi}{2}$ or	$\frac{3\pi}{2}$ ; $\frac{2\pi}{3}$ 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	$a_1 = a_2 / a_3$ $\alpha = \beta = 90^{\circ}$ $\gamma = 120^{\circ}$



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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 tis faces. The edge of the cube a is called the lattice constant.



Primitive basis vectors for the face-centered cubic lattice.

$$a_1 = \frac{a}{2} (y + z), a_2 = \frac{a}{2} (z + x), a_3 = \frac{a}{2} (x + y)$$

## 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

$$\mathbf{A} = (n_{1}, n_{2}, n_{3}), (n_{1} + \frac{1}{4}, n_{2} + \frac{1}{4}, n_{3} + \frac{1}{4}), (n_{1} + \frac{1}{2}, n_{2} + \frac{1}{2}, n_{3}), (n_{1} + \frac{3}{4}, n_{2} + \frac{3}{4}, n_{3} + \frac{1}{4}), (n_{1} + \frac{1}{2}, n_{2}, n_{3} + \frac{1}{2}), (n_{1} + \frac{3}{4}, n_{2} + \frac{1}{4}, n_{3} + \frac{3}{4}), (n_{1}, n_{2} + \frac{1}{2}, n_{3} + \frac{1}{2}), (n_{1} + \frac{1}{4}, n_{2} + \frac{3}{4}, n_{3} + \frac{3}{4})$$

$$(0, \frac{1}{2}, \frac{1}{2}) \qquad (\frac{1}{2}, 0, \frac{1}{2}) \\ (\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}) \qquad (\frac{1}{2}, \frac{1}{2}, 0) \\ \text{Tetrahedral bonding} \qquad \text{Nature of chemical bonds}$$

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# 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



CdS

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GaAs



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## Important Semiconductors: Electronics

High speed  $\implies$  low effective mass, superior mobility. High power applications  $\implies$  large bandgap. High temperature applications  $\implies$  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 divices 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.

Cosiderations:

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



## **IMPORTANT SEMICONDUCTORS: OPTOELECTRONICS**

## DETECTORS

InGaAs (Tunable Eg)	<ul> <li>Excellent material for long haul communications (at 1.55 μm).</li> <li>Can be lattice matched to InP.</li> </ul>
AlGaSb (Tunable <i>E<sub>g</sub></i> )	<ul> <li>Excellent optical properties.</li> <li>Can be used for long haul communications.</li> <li>Suffers from poor substrate availability, since it has to be grown on GaSb, whose technology is not matured.</li> </ul>
InGaAsP (Tunable Eg)	<ul> <li>Suitable for both 1.55 μm and 1.3 μm applications for long haul applications.</li> <li>Can be lattice matched to InP substrates.</li> </ul>
HgCdTe (Tunable Eg)	<ul> <li>Excellent material for long wavelength applications in night vision and thermal imaging.</li> <li>Can be used for 1.55 μm and 1.3 μm, but the technology is not as advanced as the InP based technology.</li> </ul>
$(E_g = 1.1 \text{ eV})$	<ul> <li>Indirect material with small α near the bandedge.</li> <li>Has high β<sub>imp</sub>/α<sub>imp</sub> ratio and can be used in high performance avalanche photodiodes for local area network (LAN) applications.</li> <li>Not suitable for long haul communication at λ = 1.55 μm or 1.3 μm.</li> </ul>
$Ge (E_g = 0.7 \text{ eV})$	• Indirect material with small $\alpha$ near the bandedge. • Has high $\beta_{imp}/\alpha_{imp}$ ratio and can be used for avalanche photodiodes for both local area and long distance communications.
$GaAs (E_g = 1.43 \text{ eV})$	<ul> <li>Direct gap material.</li> <li>Not suitable for high quality avalanche detectors, since α<sub>imp</sub> ≈ β<sub>imp</sub>.</li> <li>Not suited for long distance or LAN applications.</li> </ul>

## Zinc Blende and Wurtzite

	CRYSTAL		STATIC	LATTICE	
MATERIAL	STRUCTURE	BANDGAP	DIELECTRIC	Constant	DENSITY
		(eV)	CONSTANT	(Å)	$(gm-cm^{-3})$
С	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, Í	9.72	4.3596	3.166
Ge	DI	0.664, I	16.2	5.6579060	5.3234
BN	HEX	5.2, I	$\varepsilon \parallel = 5.06$	<i>a</i> = 6.6612	2.18
		,	$\epsilon^{\perp} = 6.85$	c = 2.5040	
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	$\overline{\epsilon} = 9.14$	a = 3.111	3.255
		,		c = 4.981	
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	$\epsilon = 10.4$	a = 3.175	6.095
Curt		0111,2	$\epsilon_1 = 9.5$	c = 5.158	0.070
GaP	ZB	2 272 I	11 11	5 4505	4 1 3 8
GaAs	ZB	1 4241 D	13.18	5 65325	5 3176
GaSb	ZB	0.75 D	15.10	6 09593	5 6137
InN	W	1.89.D	10.09	a = 3.5446	6.81
		1107,22		c = 8.7034	0101
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	$\epsilon \  = 8.75$	a = 3.253	5.67526
2.110		0111,2	$\epsilon_1 = 7.8$	c = 5.213	0.07020
ZnS	ZB	3 68 D	89	5 4102	4 079
ZnS	W	3 0107 D	$\overline{\mathbf{r}} = 0.6$	a = 3.8226	1.075
ZIIS	••	5.9107,D	c = 9.0	a = 5.8220 c = 6.2605	4.004
7.50	70	2 8215 D	0.1	c = 0.2003	5 766
		2.8213,D	9.1	5.0070	5.200
		2.3941,D	0.7	0.1057	3.030 9.15
CaO	K	0.84,1	- 0.02	4.089	8.15
CdS	W	2.501,D	$\varepsilon = 9.83$	a = 4.1362	4.82
G 10	70	0 50 D		c = 6./14	
CdS	ZB	2.50,D		5.818	
CdSe	W	1.751,D	$\epsilon    = 10.16$	a = 4.2999	5.81
			$\epsilon \perp = 9.29$	c = 7.0109	
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  $\varepsilon \parallel$ : parallel to *c*-axis;  $\varepsilon \perp$ : perpendicular to *c*-axis

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# 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

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

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,	TETRAHEDRA	ALLY BONDEI	MATERIALS		
V	С	Si	Ge	α-Sn	
C Si Ge	5.5i,D 2.6i,Z/W	1.1i,D 0.7-1.1	0.7-1.1i 0.74i,D		
α-Sn III-V	N	Р	As	0.09,D Sb	i: Indirect gap
B Al Ga In	3.8,W 5.9,W 3.5,W 0.9,W	2.0i,Z 2.5,Z 2.4i,Z 1.4,Z	1.5i,Z 2.2,Z 1.5,Z 0.41,Z	1.7,Z 0.81,Z 0.24,Z	Z: Zinc Blende W: Wurtzite R: Rocksalt
II-VI	0	S	Se	Te	O: Orthorhombic
Zn Cd Hg	3.4,W 1.3i,R 2.2,O/Rh	3.6,Z/W 2.5,Z/W 2.3,T	2.8,Z/W 1.8,Z/W 06,Z	2.4,Z 1.6,Z 3,Z	Rh: Rhombohedral T: Trigonal OR: Orthorhombic
I-VII	F	Cl	Br	Ι	distorted rocksalt
Cu Ag	2.8i,R	3.4,Z 3.2i,R	3.1,Z 2.7i,R	3.1,Z 3.0,W	M: Monoclinic

## Bandgaps (in eV) of some semiconductors

IV-VI compounds

	1						
IV-VI	0	S	Se	Te			
Ge Sn Pb	2.0,i	1.7,OR 1.1,OR 0.29,R	1.1,OR 0.9,OR 0.15,R	0.15,R 2.1,R 0.19,R			
Group	Group VI elements						
VI	S	Se	Te				
	3.6,0	1.9i,T 2.5,M	0.33,T				
Group V elements							
V	Р	As	Sb	Bi			
_	.33,0	.17,Rh	.10	.015			

Non-tetrahedral bonded materials

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