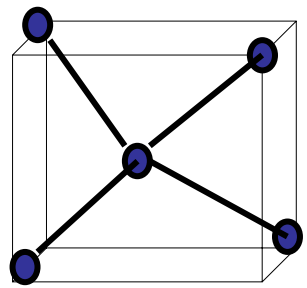
Elements Constituting Semiconductors

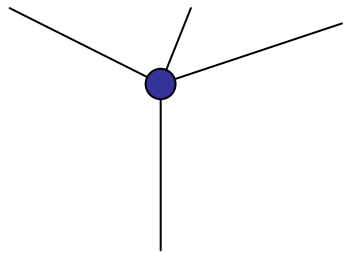
Ib s1	IIb s2	III s2 p1	IV s2 p2	V s2 p3	VI s2 p4	VII s2 p5
		B	C	N	O	F
		Al	Si	P	S	Cl
Cu	Zn	Ga	Ge	As	Se	Br
Ag	Cd	In	Sn	Sb	Te	I

A Elementary Semiconductors

Group IV	Gap energy Eg (eV) @ RT
C, diamond	5.5
Si	1.1
Ge	0.66
α-Sn	0

- **covalent bonding**
- 2 electrons per bond
- 1 electron per bond per atom
- max 4 bonds: **Coordination 4**
- **tetrahedral arrangement**
- **bond angle = 110 °**





Other elementary semiconductors

As, P 3 fold- coordinated

S, Se 2-fold coordinated

of marginal importance

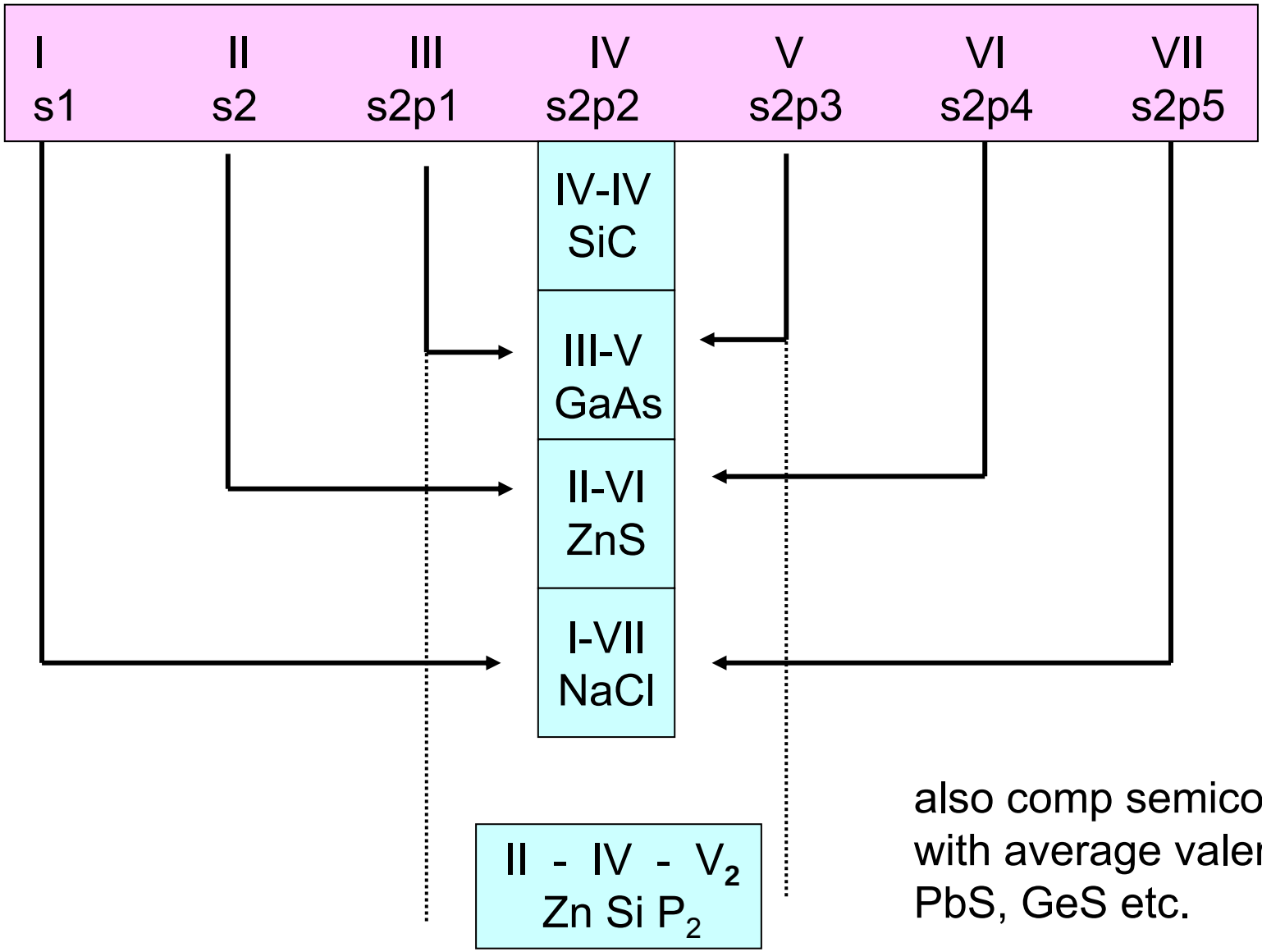
Compound Semiconductors

Binary, ternary or quaternary compounds with

- s, p valence electrons
- average # of valence electrons per atom = 4
- **primaryly covalent bonds**
- **tetrahedral coordination**
- **structures comparable to Si, Ge**

Examples: GaAs, ZnS, AlN, $CuInSe_2$

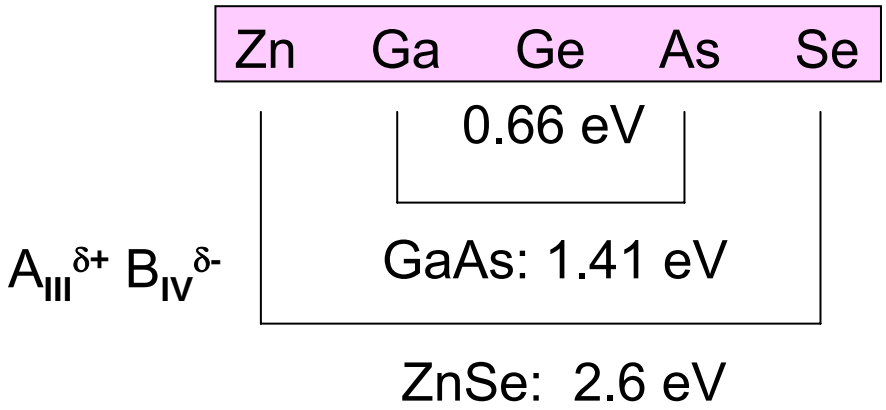
B Compound Semiconductors



also comp semiconductors with average valence 5: PbS, GeS etc.

Bonding in Binary Semiconductors

Partially ionic bond increases energy gap



I-VII rein ionisch, NaCl, CsCl structure; insolators: NaF (11.5 eV); NaCl (9 eV)

C Examples

a) IV-IV

SiC

+ 250 different crystal structures: Polytypes
all based on Si-C_4 viz. C-Si_4 tetrahedra

$2.5\ eV \leq E_g \leq 3.4\ eV$

application in the area of high power/high frequency

b) III-V semiconductors

	Eg (eV)		cryst str.
GaN	3.40	d	Wu/Zb
GaP	2.27	i	Zb
GaAs	1.41	d	Zb
GaSb	0.70	d	Zb
AlN	6.20	d	Wu
AlP	2.50	d	Zb
AlAs	2.16	d	Zb
AlSb	1.3	d	Zb

c) II-VI semiconductors

	Eg (eV)		cryst str.
ZnO	3.3	d	Wu
ZnS	3.68	d	Zb
ZnS	3.8	d	Wu
ZnSe	2.7	d	Zb
ZnTe	2.3	d	Zb
CdS	2.5	d	Zb
Cdse	1.8	d	Zb
CdTe	1.4	d	Zb

All important for optical applications
because they have direct band gaps

d) Chalcopyrite semiconductors

I-III-VI_2	$CuInSe_2$ (CIS) $CuInS_2$	E_g ~ 1.5 eV for thin film solar cells

e) IV-VI semiconductors; average valency = 5

GeS, GeSe, PbS, PbSe, HgS, HgSe

on average Eg ≤ 0.2 eV; for IR detector applications

Zusammenfassung I.1

- HL rekrutieren sich aus Elementen mit s,p Valenzelektronen
- Hl sind vorwiegend kovalent gebunden; maximale Koordinationszahl = 4 für HL mit 4 Valenzelektronen in 4 Valenzorbitalen
- starke kovalente (+ part. Ionisch) Bindung
  → starke Aufspaltung bindend-antibindend → **Energielücke**
- Gruppe IV: C, Si, Ge, α-Sn, indirekte BL
- III-V HL: GaAs, AlN ……
- II-VI HL: ZnS, ZnO, ….
- I-II-VI2 HL: Chalcopyrite $CuInS_2$

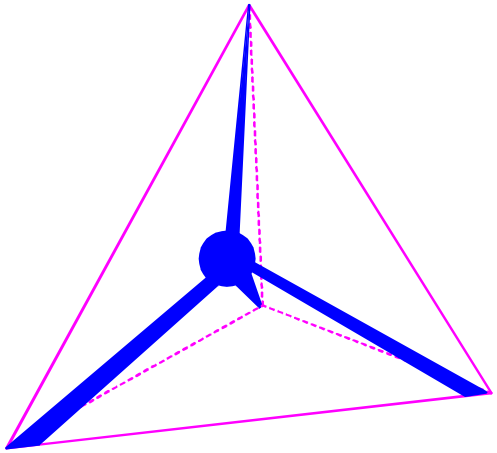
direkte Energielücke

Legierungen decken den sichtbaren Bereich des Spektrums ab

380…..800 nm
3.25… 1.55 eV

1.5 mm 1.20 eV
IR für Glasfaserkommunikation

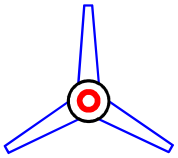
Forming the most important crystal structures from their elemental building blocks



step by step

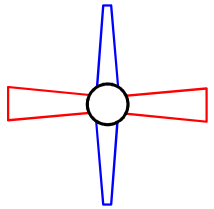
The Diamond and the Zincblende Structure

corner view: C_{3v}

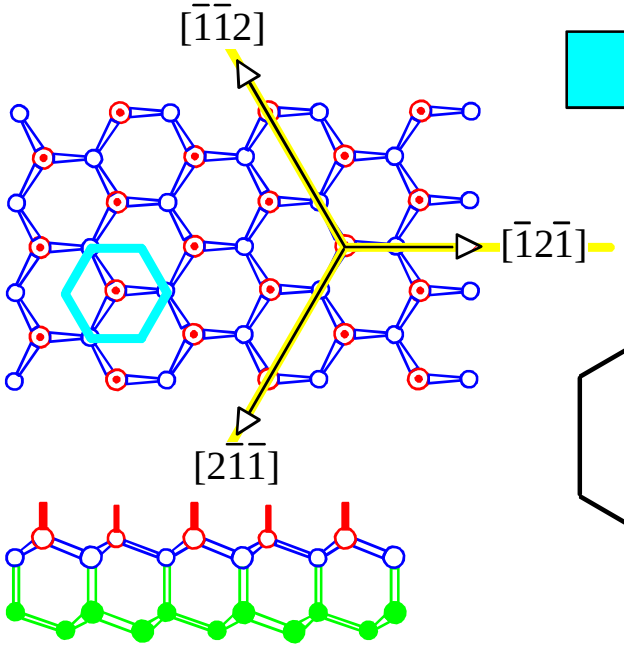


Tetrahedral building blocks

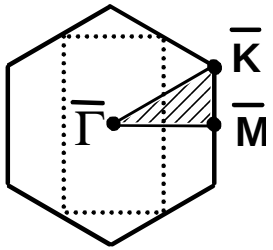
edge view: C_{2v}



View towards (111) direction

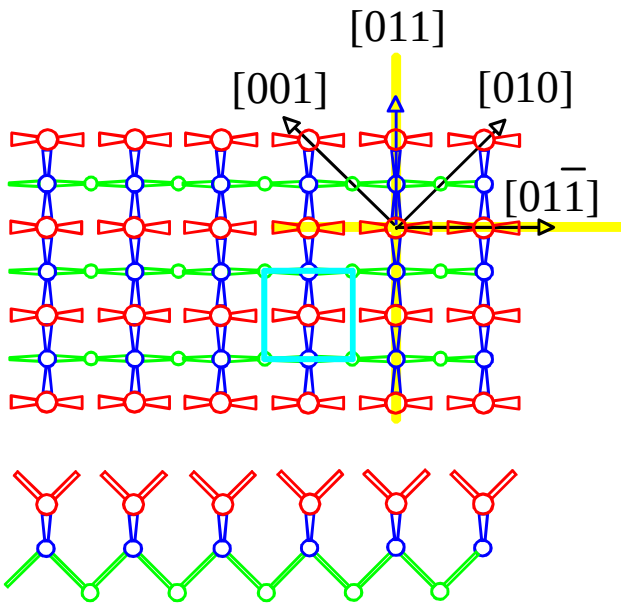


1x1

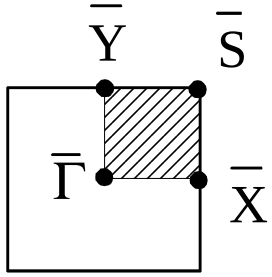


surface Brillouin zone

View towards (100) direction



1x1

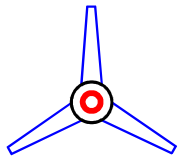


surface Brillouin zone

Zincblende and Wurtzite

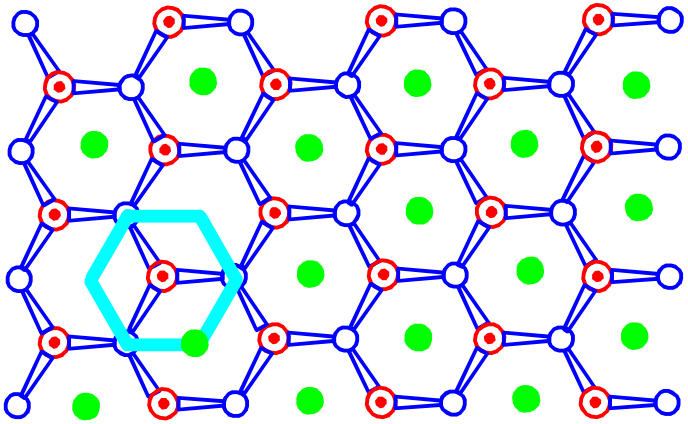
Tetrahedral building blocks

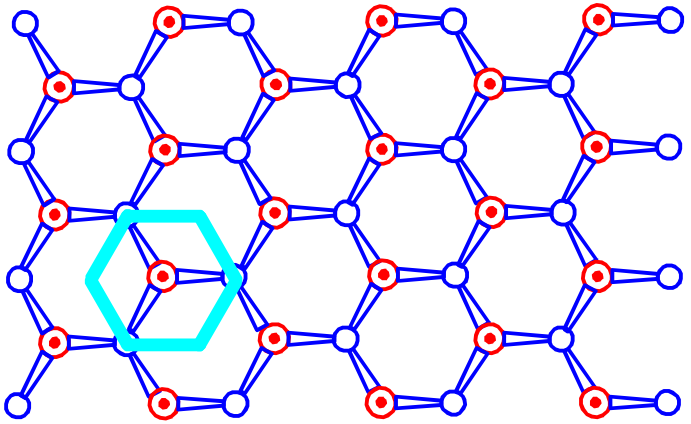
corner view: C_{3v}

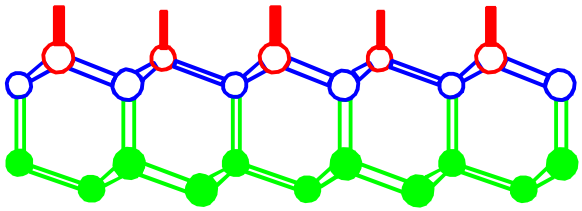


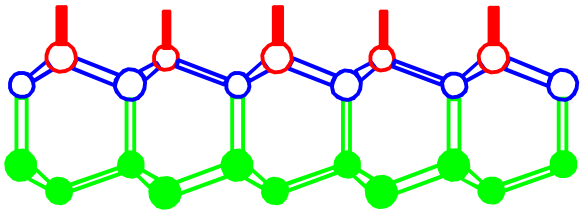
Cubic crystal symmetry

Hexagonal crystal symmetry



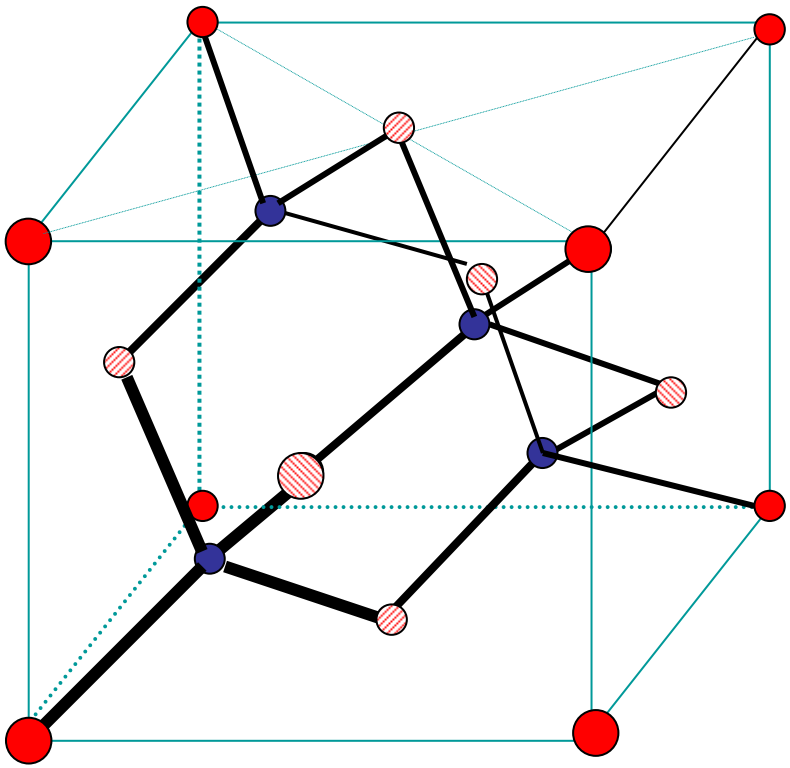






Diamond/Zinkblende Crystal Structure

diamond structure: all atoms the same, e.g. Si
ZB: red Ga, blue As



Nearest neighbor atoms along space diagonal

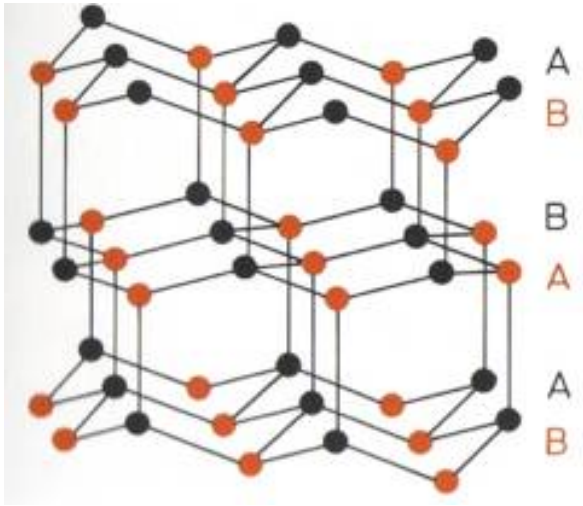
Nearest neighbor (nN) distance = ¼ space diagonal

Face centered cubic (fcc) with two atom basis

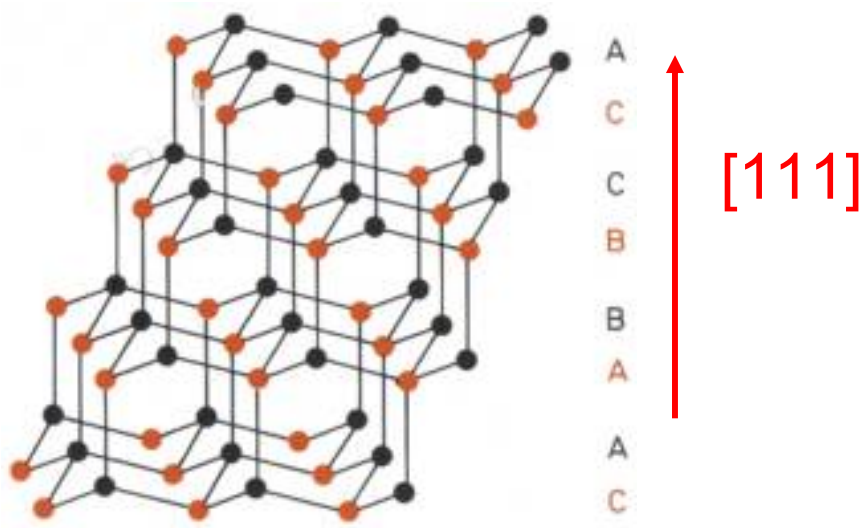
Number of atoms = 8/8 + 6/2 + 4 = 8 atoms per fcc unit cell

Comparison WZ-ZB

WZ

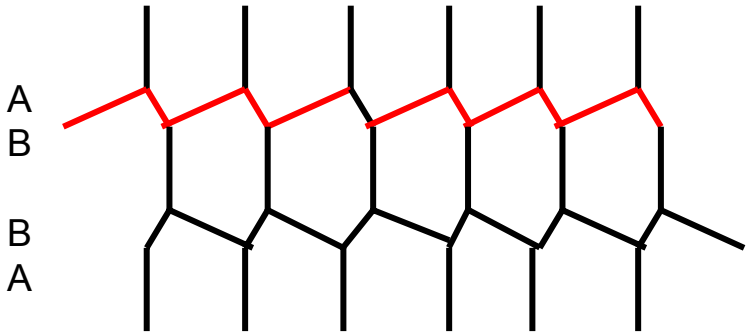


ZB

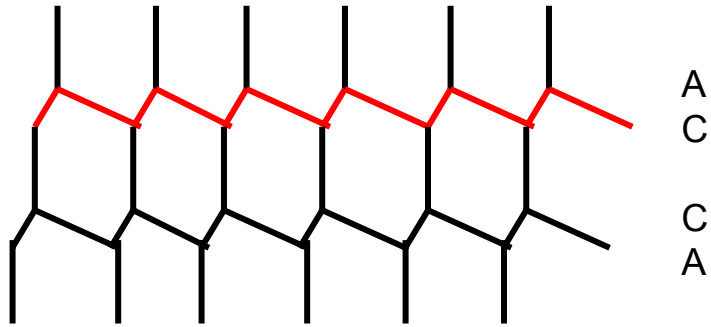


structural motive: tetrahedra

structural theme: double layers



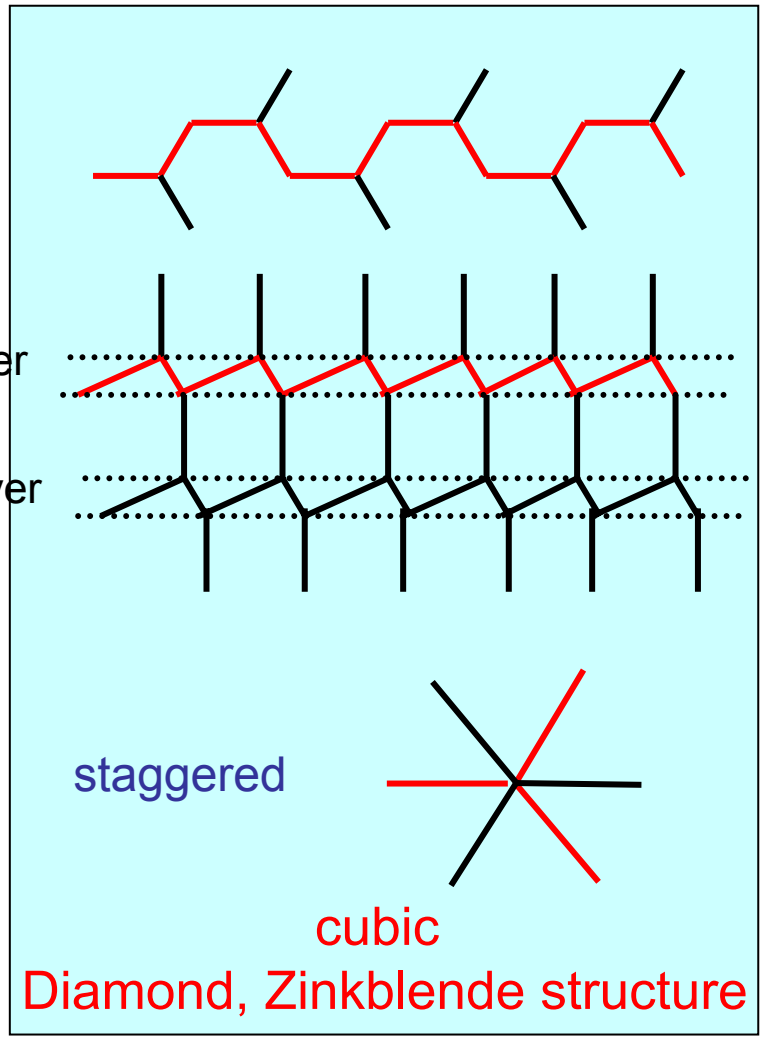
Tetrahedra are eclipsed

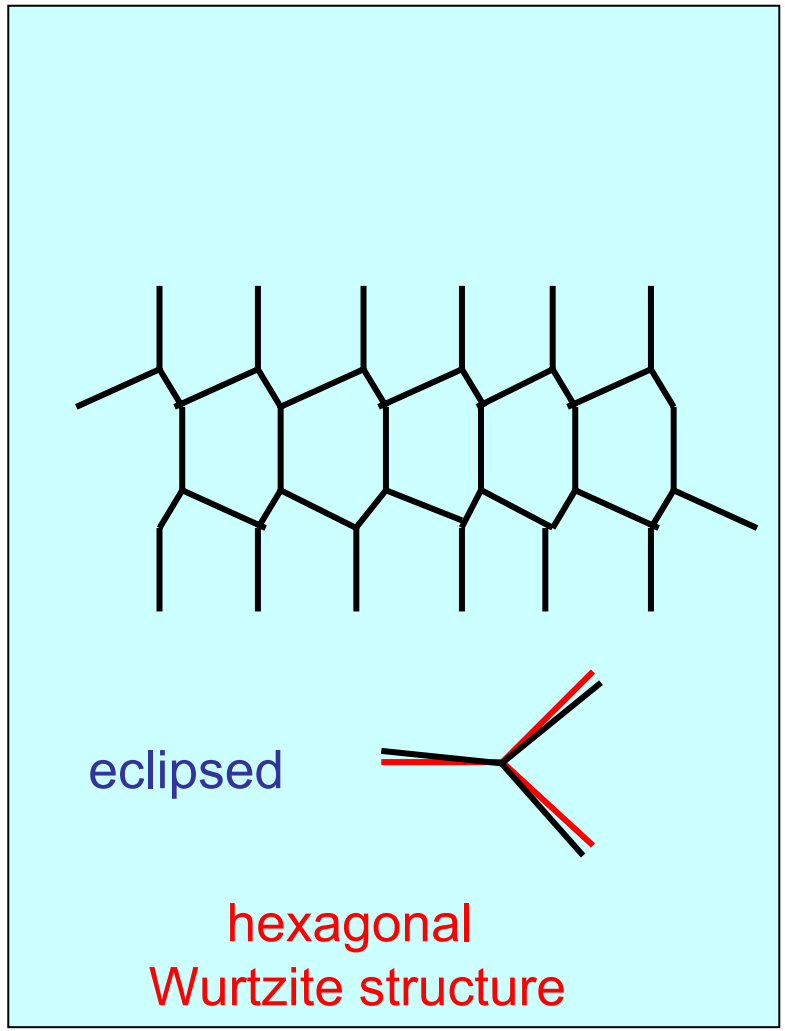


Tetrahedra are staggered

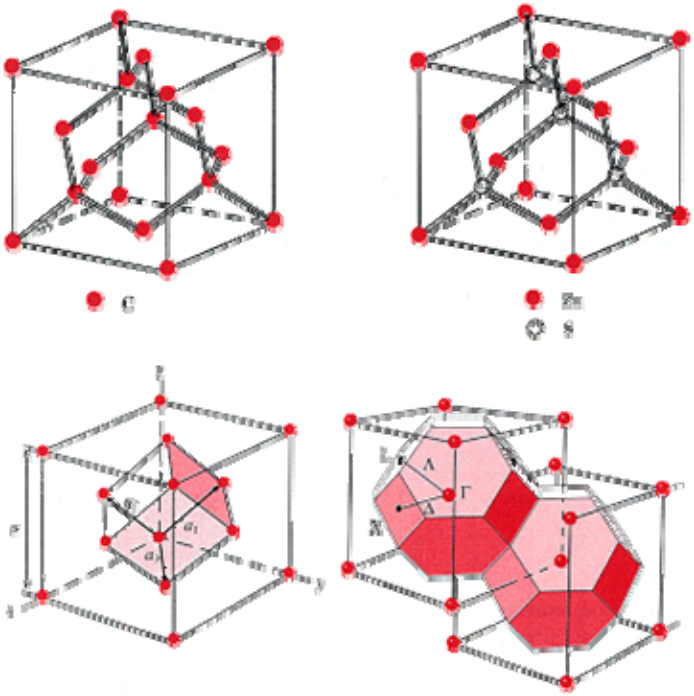
Crystal Structures of SC

Structural theme. A-B double layer

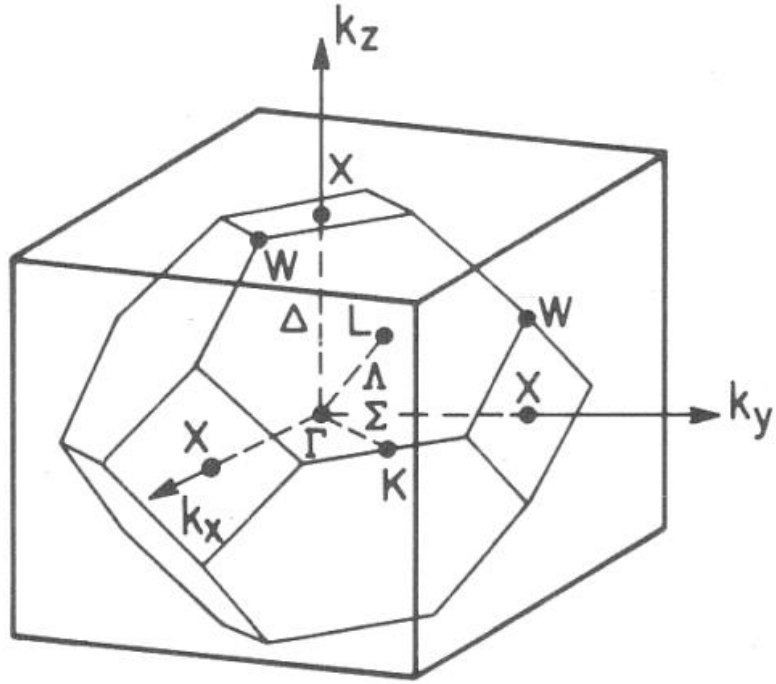




Real and reciprocal lattice of diamond/ZB structure

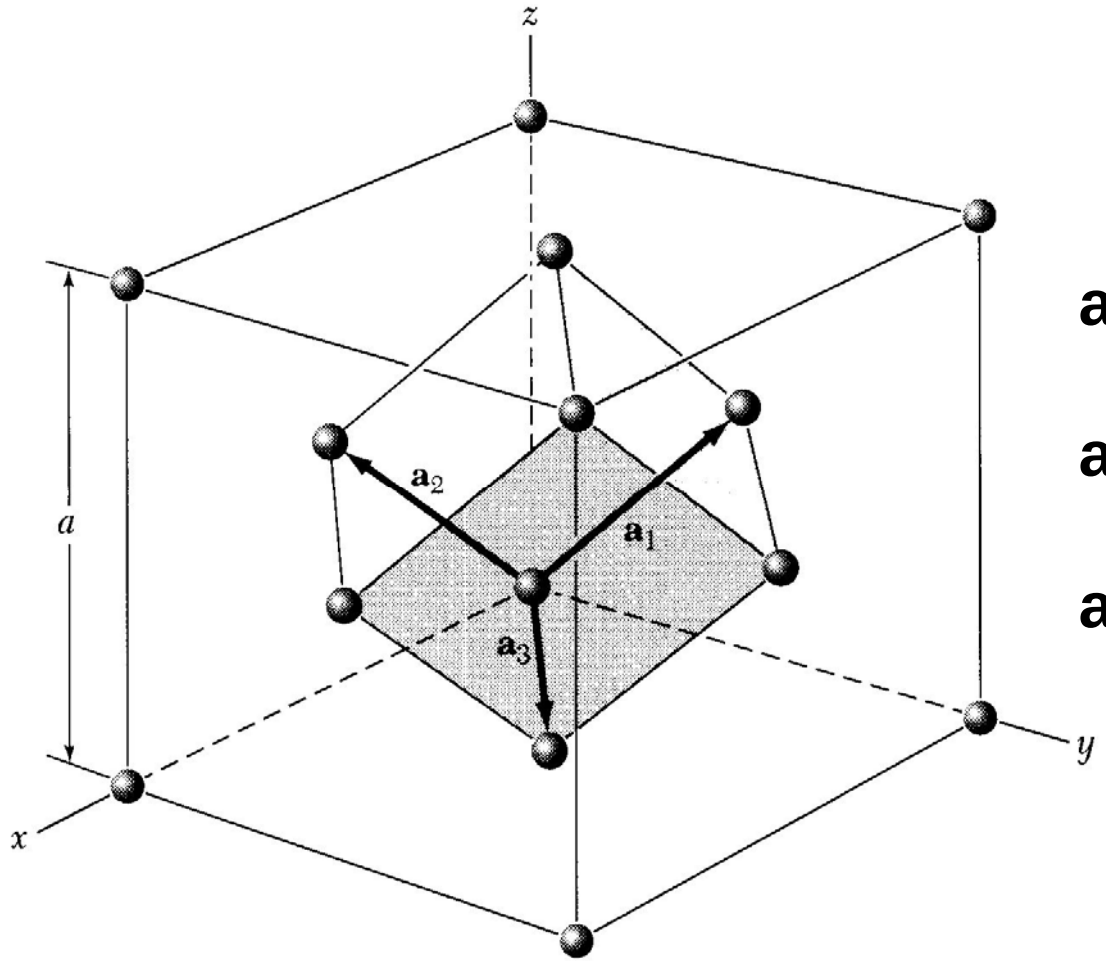


Face centered cubic



Body centered cubic

Primitive unit cell of diamond and ZB structure

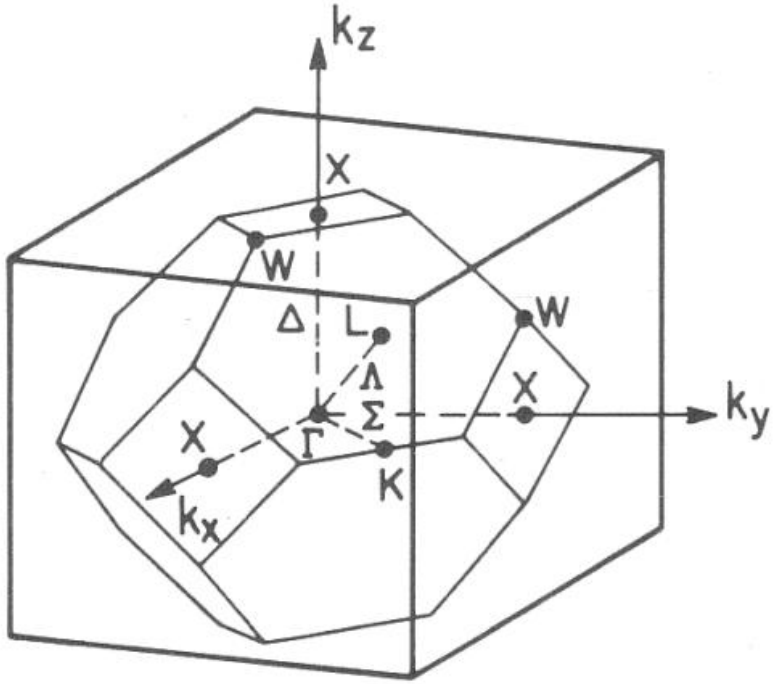


$\mathbf{a}_1$ = 1/2 [010] +1/2 [001]

$\mathbf{a}_2$ = 1/2 [100] +1/2 [001]

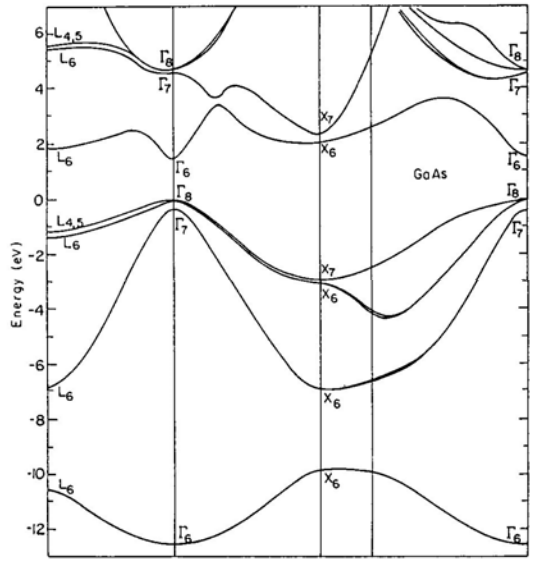
$\mathbf{a}_3$ = 1/2 [010] +1/2 [100]

Band structures of Si and GaAs



Brillouine-Zone of Diamond/ZB structure

GaAs



Si