

3.46 PHOTONIC MATERIALS AND DEVICES

Lecture 2: Optical Materials Designs Part 2

Lecture

Notes

Materials Property Design

“Property Maps”

Meoser-Pearson, *Acta Crystallographica*, **12**, 1015 (1959).

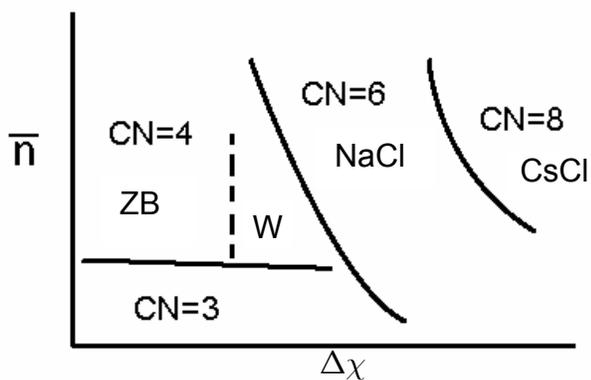
2-dimensional: \bar{n} vs. $\Delta\chi$

Average principal quantum number (\bar{n})
vs. electronegativity difference ($\Delta\chi$)

Villaro, J., “Less Common Metals,” **92**,
215 (1983).

3-dimensional: r_{AB} vs. N_{be} vs. $\Delta\chi$

Orbital radii vs. number of valence
electrons vs. electronegativity difference



CN: Coordination Number

ZB: Zincblende

W: Wurtzite

Structures of Simple Ionic Crystals		
Minimum Radius Ratio	Coordination Number	Coordination Symmetry
0	2	linear
0.155	3	Planar
0.225	4	Tetrahedral
0.414	6	Octahedral
0.732	8	cubic
1.000	12	

Materials (semiconductors)

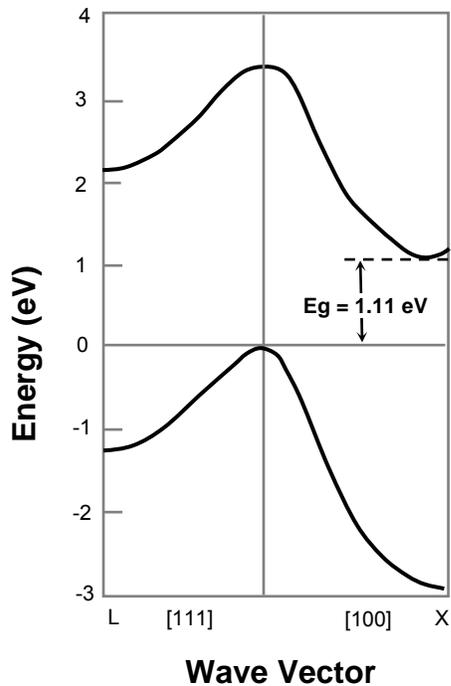
Elemental: Si, Ge

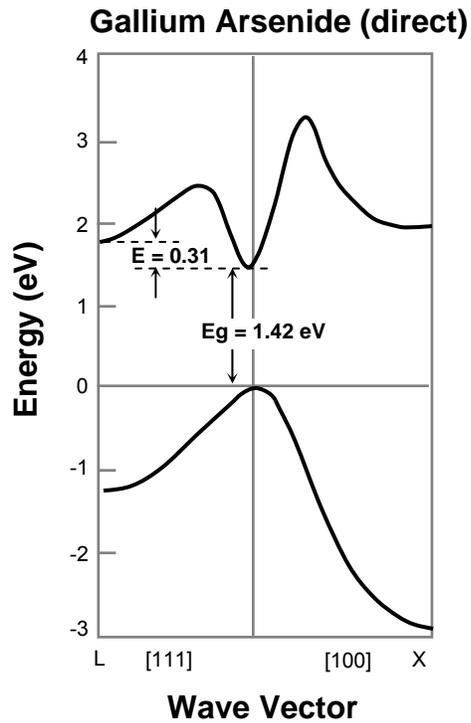
Binary compound: GaAs, InP

Ternary alloy: $\text{Al}_x\text{Ga}_{1-x}\text{As}$

Quarternary alloy: $\text{In}_{1-x}\text{Ga}_x\text{As}_{1-y}\text{P}_y$

Silicon (indirect)

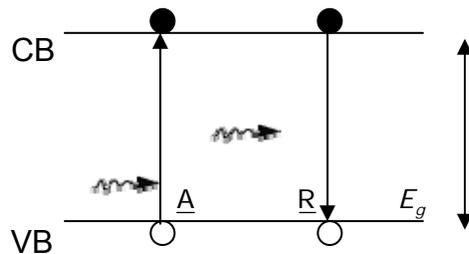




Energy band: a set of closely spaced energy levels of atoms in solid that represent the entire system.

Valence band: highest filled band.

Conduction band: lowest empty band.



Absorption can create e^-h^+

e^-h^+ Recombination can create a photon

“Bandgap Wavelength”

Free space wavelength of photon energy E_g

$$\lambda_g = \frac{hc_0}{E_g}$$

wavevector: \vec{k}
(crystal) momentum: \vec{p}

$$\vec{p} = \hbar\vec{k}$$

Effective mass

@ band extrema (conduction, valence)

$$E = E_c + \frac{\hbar^2 k^2}{2m_c^*}$$

$$E = E_v - \frac{\hbar^2 k^2}{2m_c^*}$$

m_0 = rest mass of e^-
= 9.1×10^{-31} kg

Average value m^* for Si, GaAs

	$\frac{m_c^*}{m_0}$	$\frac{m_v^*}{m_0}$
Si	0.33	0.5
GaAs	0.07	0.5

Direct gap (Si)

No change in momentum for CB \leftrightarrow VB electronic transition.

Indirect gap (Si)

Band extrema at different \vec{k}
Change in \vec{k} , \vec{P} required

Compound semiconductors

III-V compounds

f_i = fractional ionic character

CE = cohesive energy
= $\Delta G_{\text{sublimation}}$ (neutral atom, STP)

$$\frac{f_i}{CE} \quad \text{CE (kcal/mole)}$$

	N	P	As	Sb
B	$\frac{.256}{-293}$			
Al		$\frac{.307}{-170}$	$\frac{.274}{-157}$	
Ga		$\frac{.327}{-152}$	$\frac{.310}{-135}$	$\frac{.261}{-118}$
In		$\frac{.421}{-133}$	$\frac{.357}{-126}$	$\frac{.321}{-108}$

\uparrow CE
 \leftarrow

Lecture

Compound	Lattice Constant (Å)	Density (gm cm ⁻³)	Melting Point (K)	Debye Temperature ^(a) (K)	Coefficient of Thermal Expansion ^(b) 10 ⁻⁶ /°C	Thermal Conductivity ^(a,b) (Wcm ⁻¹ K ⁻¹)
AIP	5.467	2.40	2823	588	4.5	0.9
AlAs	5.660	3.70	2013	417	4.9	0.8
AlSb	6.136	4.26	1338	292	4.0	0.57
GaP	5.4512	4.138	1740	456	4.5	0.77
GaAs	5.6532	5.3161	1513	344	6.86	0.46
GaSb	6.0959	5.6137	985	266	7.75	0.39
InP	5.8687	4.81	1335	321	4.75	0.68
InAs	6.0583	5.667	1215	249	4.52	0.273
InSb	6.4794	5.7747	800	203	5.37	0.166

Elastic Compliances in Units of 10⁻¹² cm² dyne⁻¹

Compound	S ₁₁	S ₁₂	S ₄₄
AIP	1.090	-0.350	1.630
AlAs	1.070	-0.320	1.840
AlSb	1.696	-0.562	2.453
GaP	0.973	-0.298	1.419
GaAs	1.176	-0.365	1.684
GaSb	1.582	-0.495	2.314
InP	1.650	-0.594	2.170
InAs	1.945	-0.685	2.525
InSb	2.443	-0.863	3.311

Deformation Potential Constants

Compound	a(eV)		b(eV)	d(eV)
	Direct gap	Indirect gap		
AIP				
AlAs				
AlSb	-5.9	2.2	-1.35	-4.3
GaP	-9.6		-1.65	-4.5
GaAs	-9.77		-1.70	-4.55
GaSb	-8.28		-2.0	-4.7
InP	-6.35		-2.0	-5.0
InAs	-6.0		-1.8	-3.6
InSb	-7.7		-2.0	-4.9

Lecture

SiO₂ $E_g = 10.2\text{eV}$

Main contribution to n for silicates is the polarizability of the oxygen.

$\chi \uparrow$ as \bar{n} (cation) \uparrow
e.g., PbO

(flint glass) is yellow (absorbs in violet)

anions are more polarizable than cations

$F < OH < Cl < O < S < Se < Te$

BeF₂ for UV transmission

Fluorozirconates for long λ

ZrF₄, BaF₂, LaF₂

Long λ loss < SiO₂

Notes