Review:

Bonds and Bands

Basic semiconductor physics

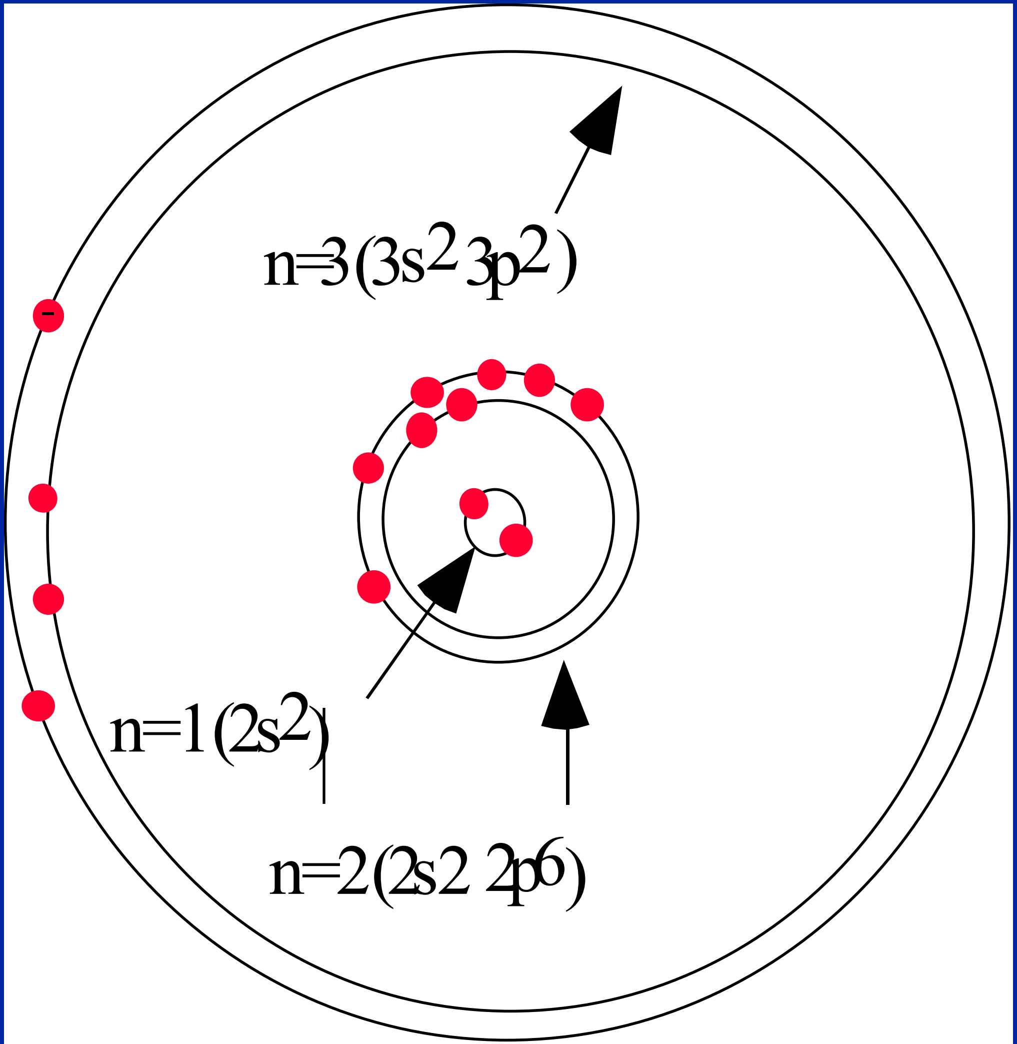
Semiconductor Materials

- Silicon electronic structure
- Silicon crystal structure
- Other atoms
- Zinc Blende and wurtzite crystal structures

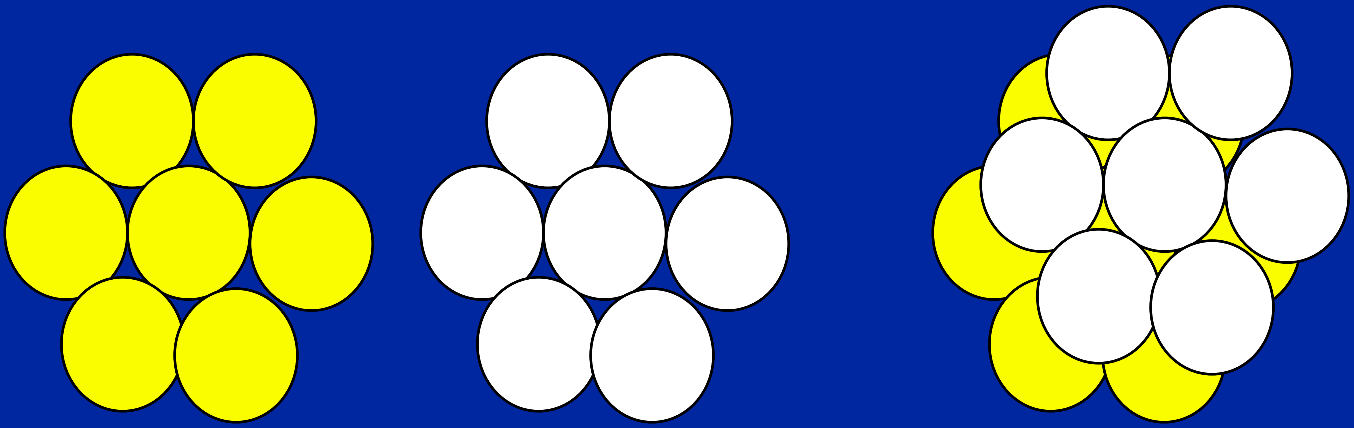
Time line for Semiconductor Materials

- Germanium Decade 1947 -1958
- Silicon Age 1962 -
- GaAs Age 1970 -
- Wide band Semiconductor Age 1990-
- Polymers ? Amorphous materials? Rare earth?

Electronic configuration of Si

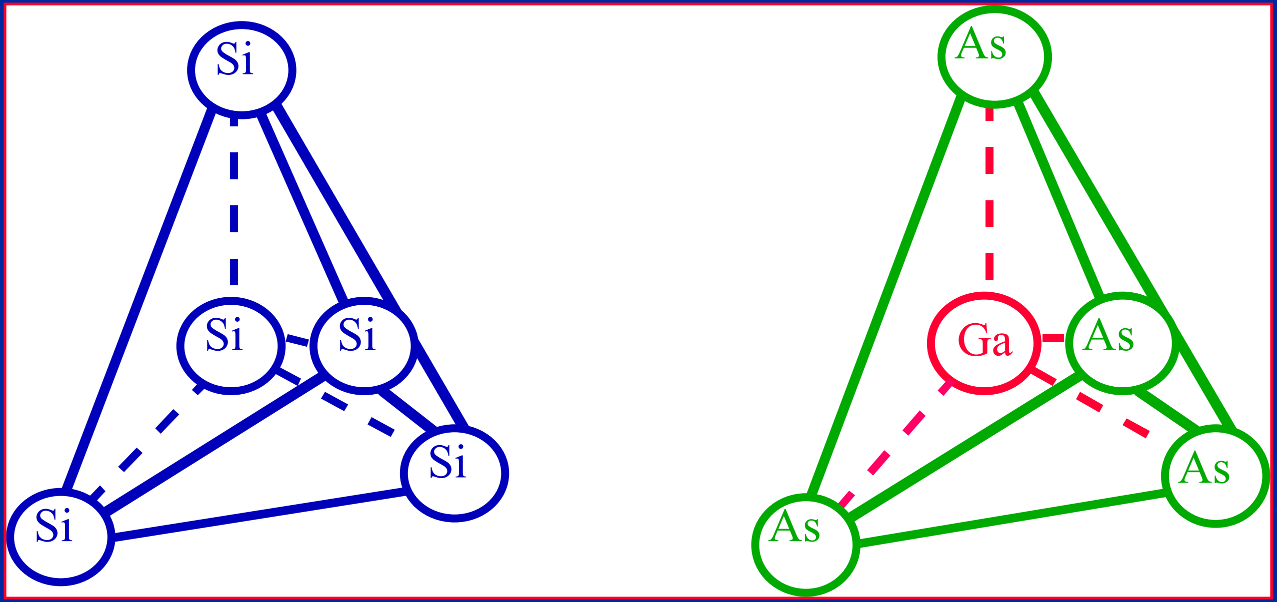


Atoms in a Crystal Touching and Unit Cell

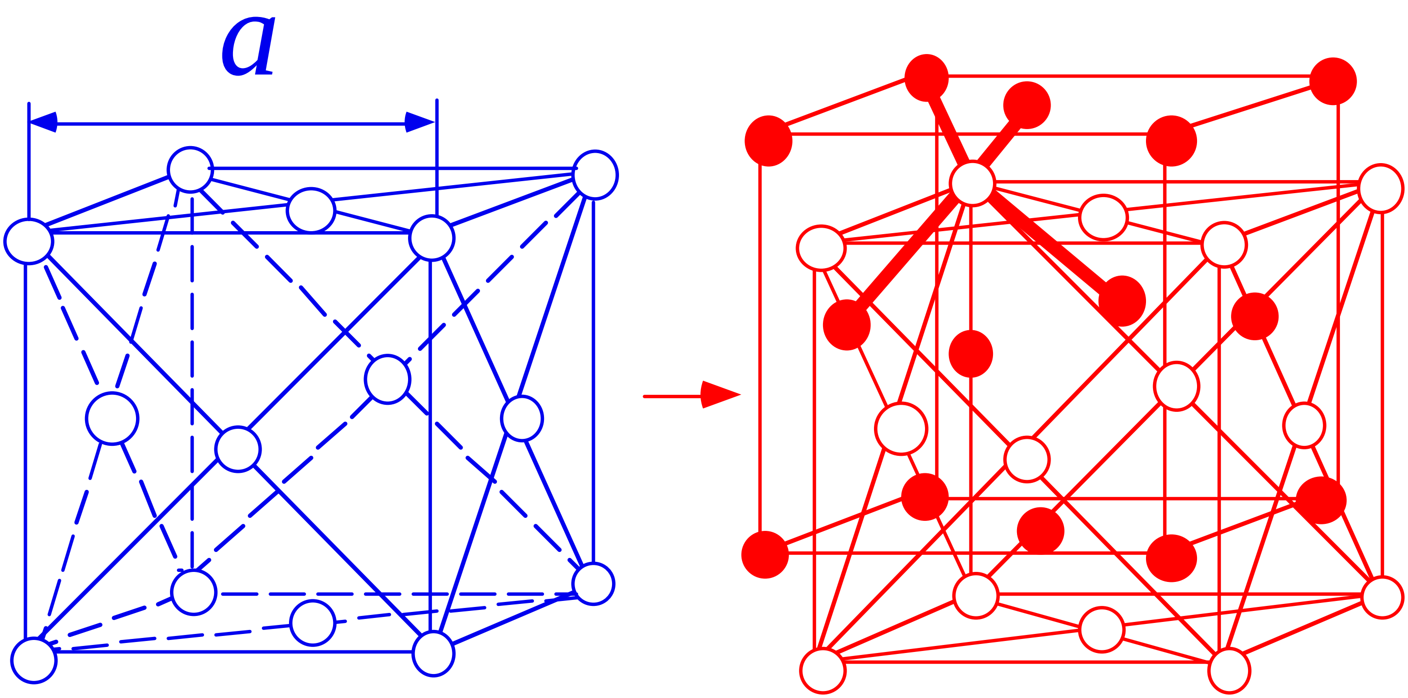


http://www.youtube.com/watch?v=JRePI-8QPKg&NR=1

Tetrahedral bonding configuration



Face Centered Cubic and Diamond Crystal Structure



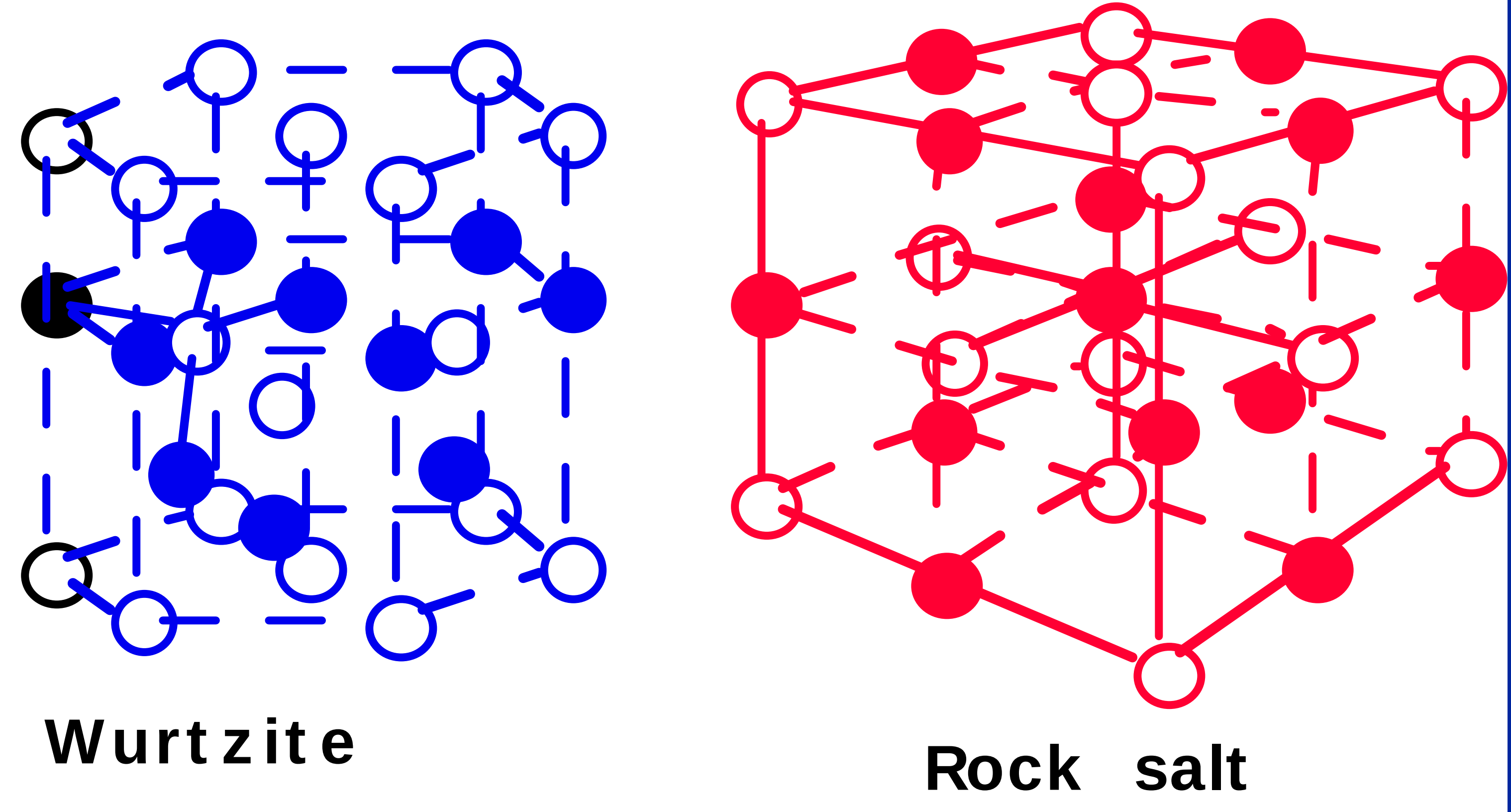
How to emulate silicon?

Mix and match atoms having the same number of valence electrons (8) and form compounds having tetrahedral bonding

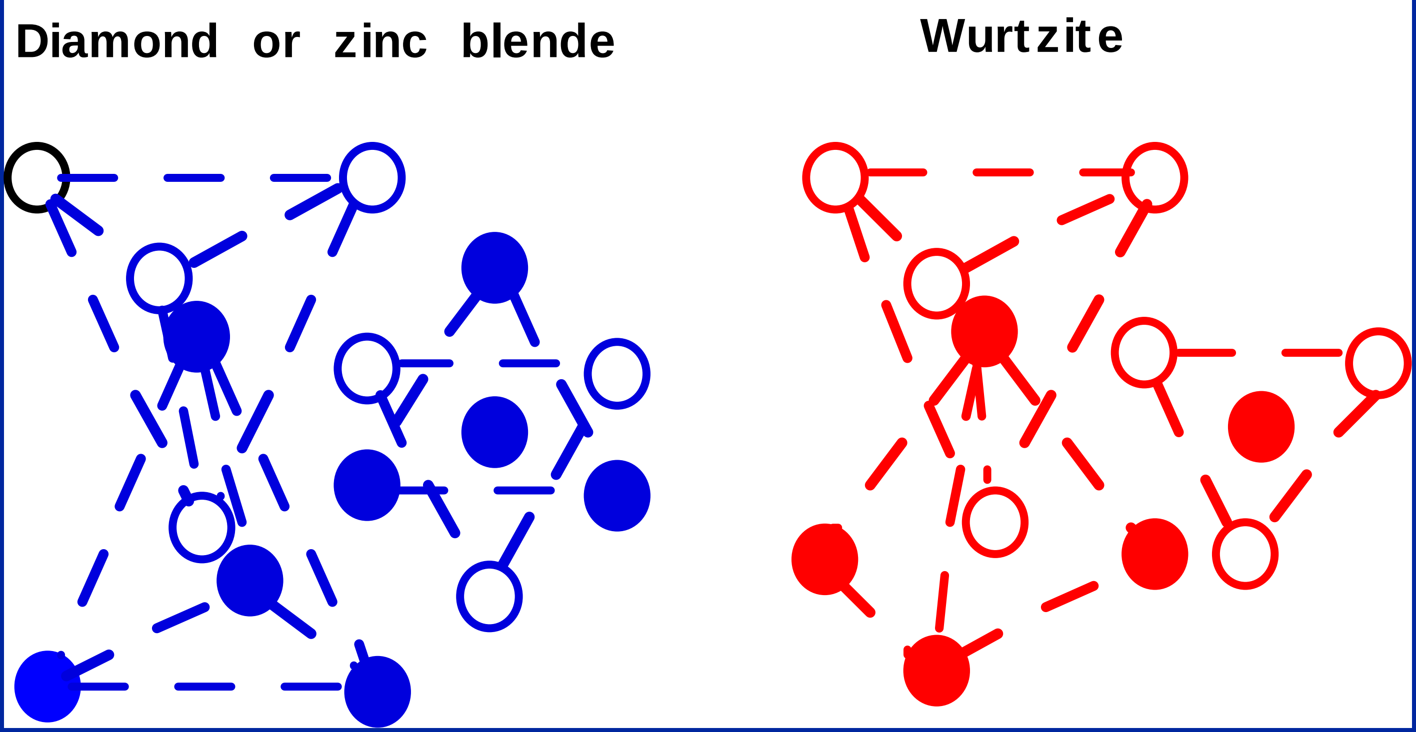
Group III - 3 valence electrons - and group V - 5 valence electrons (III-V, III-N)

Group II - 2 valence electrons - and group VI - 6 valence electrons (II-VI)

Other crystal structures



Wurtzite and zinc blende



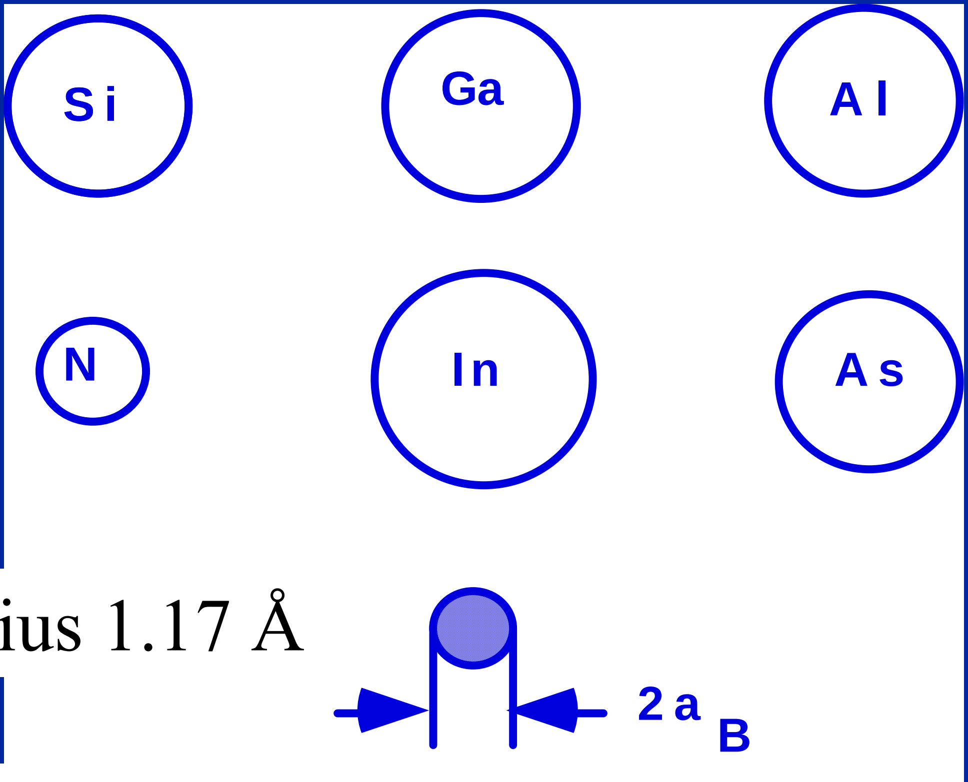
Crystal Structures on the WEB (can be rotated)

- http://www.ibiblio.org/e-notes/Mview/Packed.htm
- http://www.ibiblio.org/e-notes/Cryst/Cryst.htm

(might need additional software to see all features)

- See also
- Making Matter. The atomic structure of materials" by *M. Hewat*,
  "Materials Science. Introduction to Concepts"
  by *Simon Toh* and
  Teaching and Education in Crystallography.

Atomic dimensions



Silicon radius 1.17 Å

$a_B = 0.52$ Å

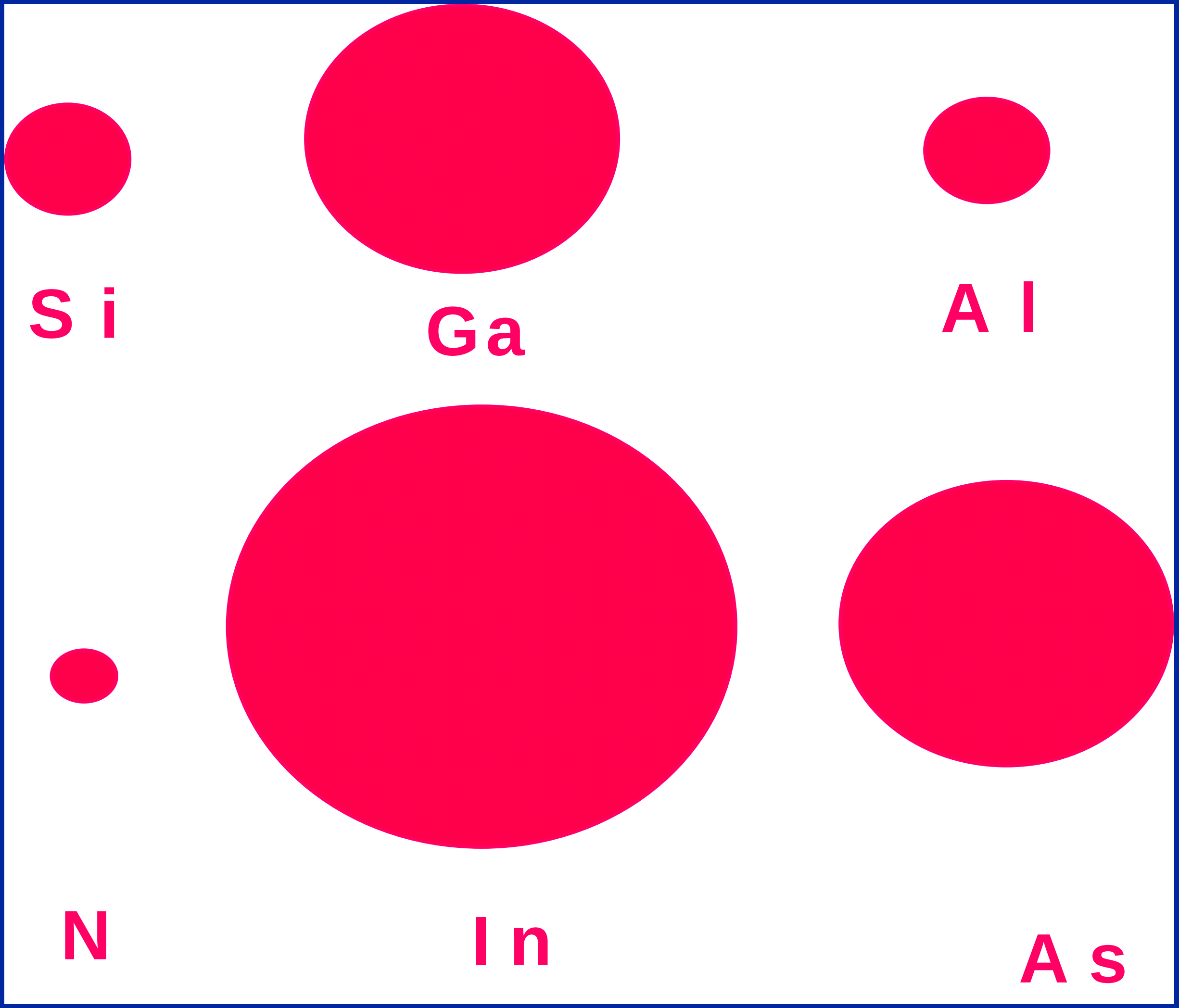
shurm@rpi.edu

Atomic radii

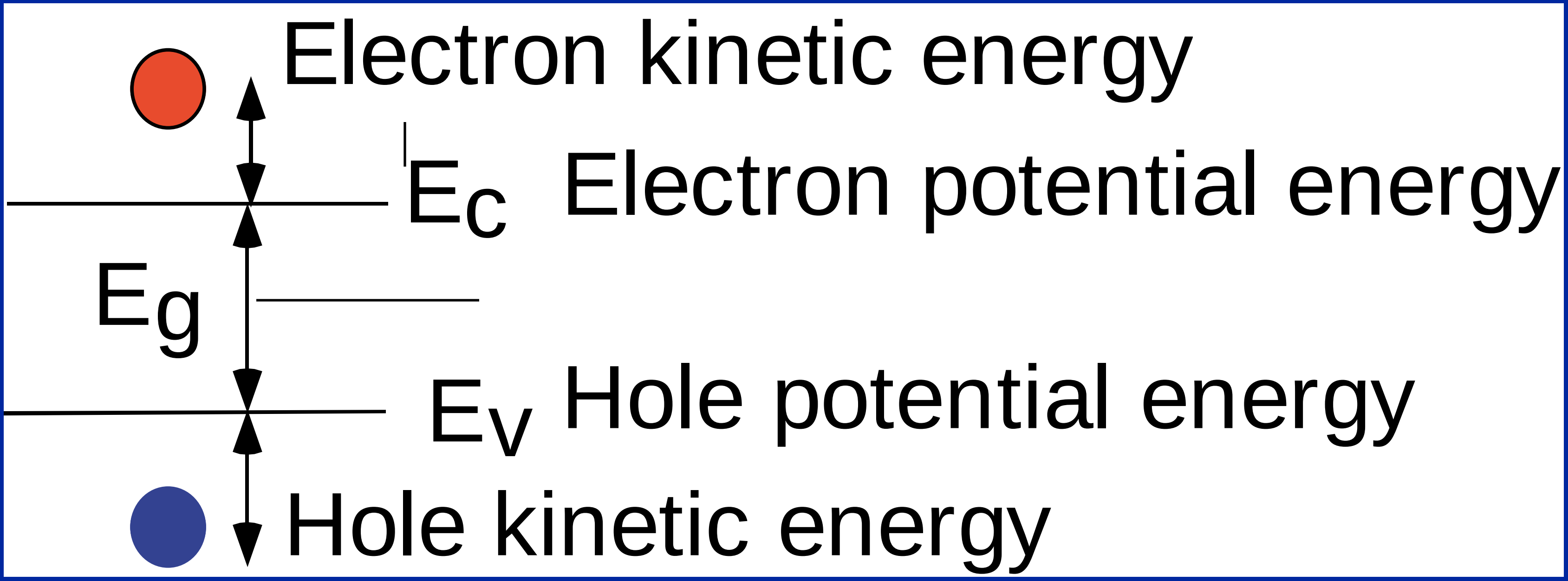
Element	Tetrahedral radius (Å)
Al	1.26
As	1.18
B	0.88
Bi	1.46
C	0.77
Ga	1.26
Cd	1.48
Ge	1.22
Hg	1.48
In	1.44
Mn	1.27
N	0.70
P	1.10
Sb	1.36
Si	1.17
Sn	1.40
Te	1.47
Zn	1.31

From M. Shur, Introduction to Electronic Devices, Wiley (1990)

Atomic masses represented by relative sizes



Band diagram basics
Real Space



Electron kinetic energy

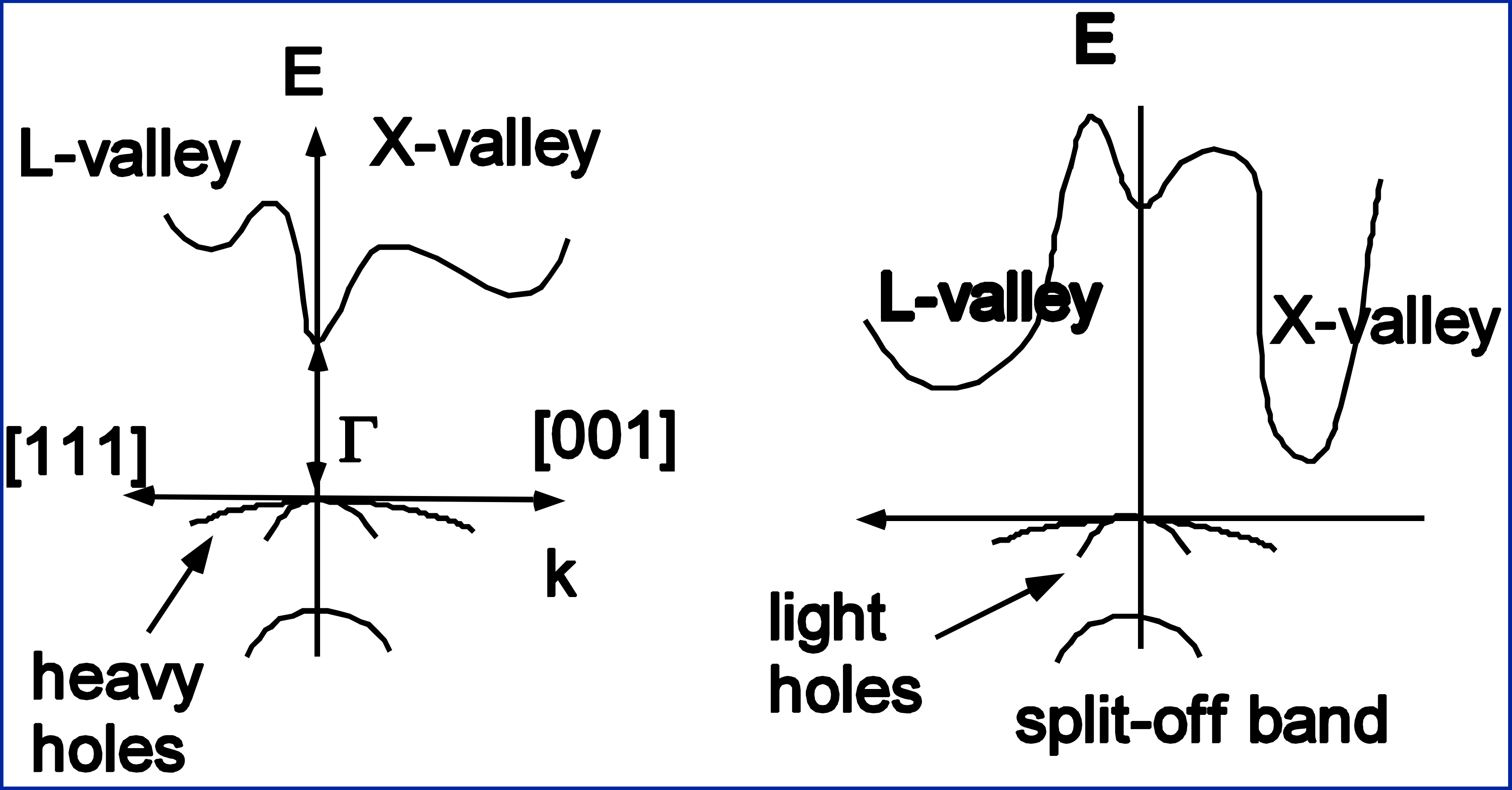
E_c Electron potential energy

E_g

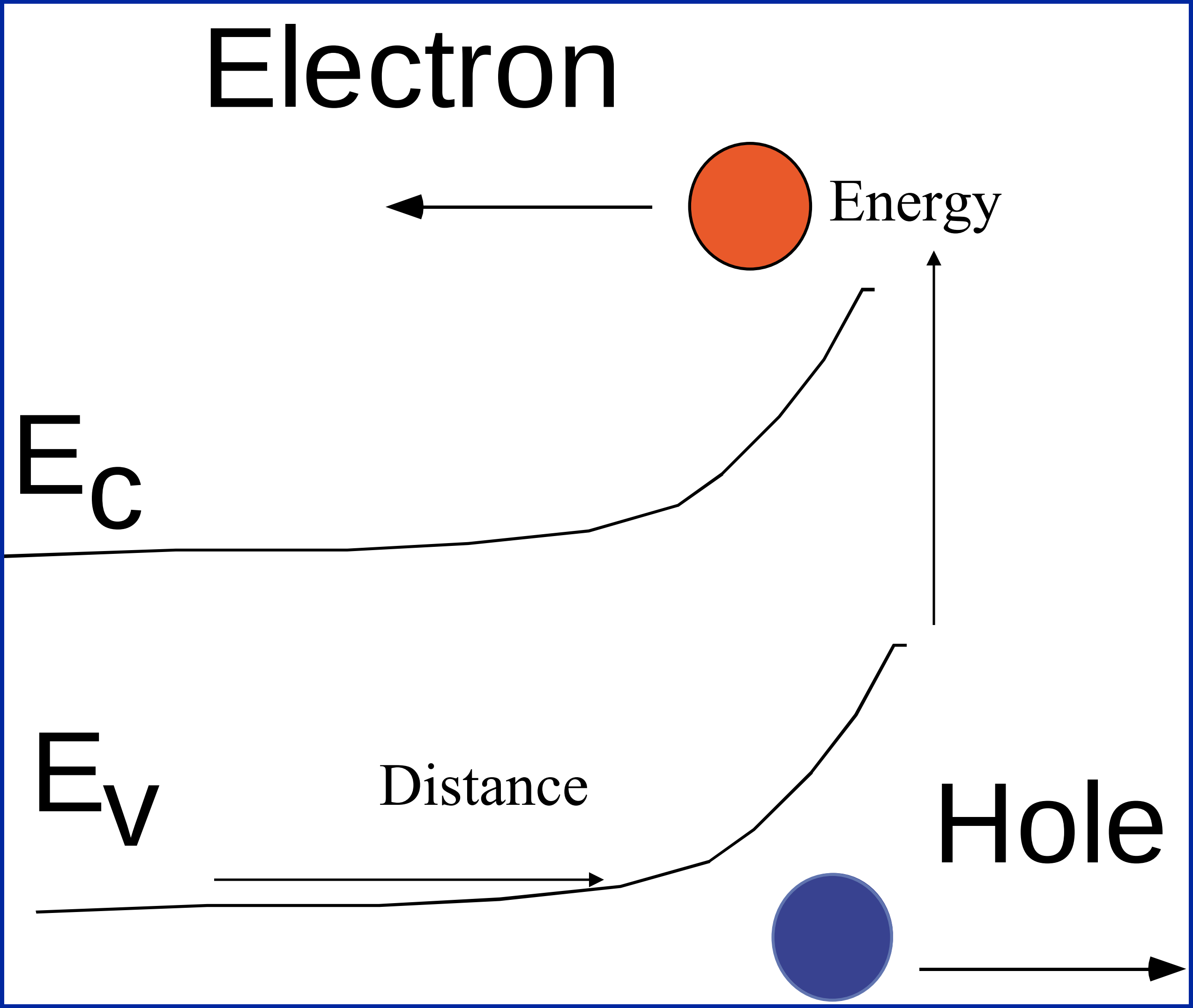
E_V Hole potential energy

Hole kinetic energy

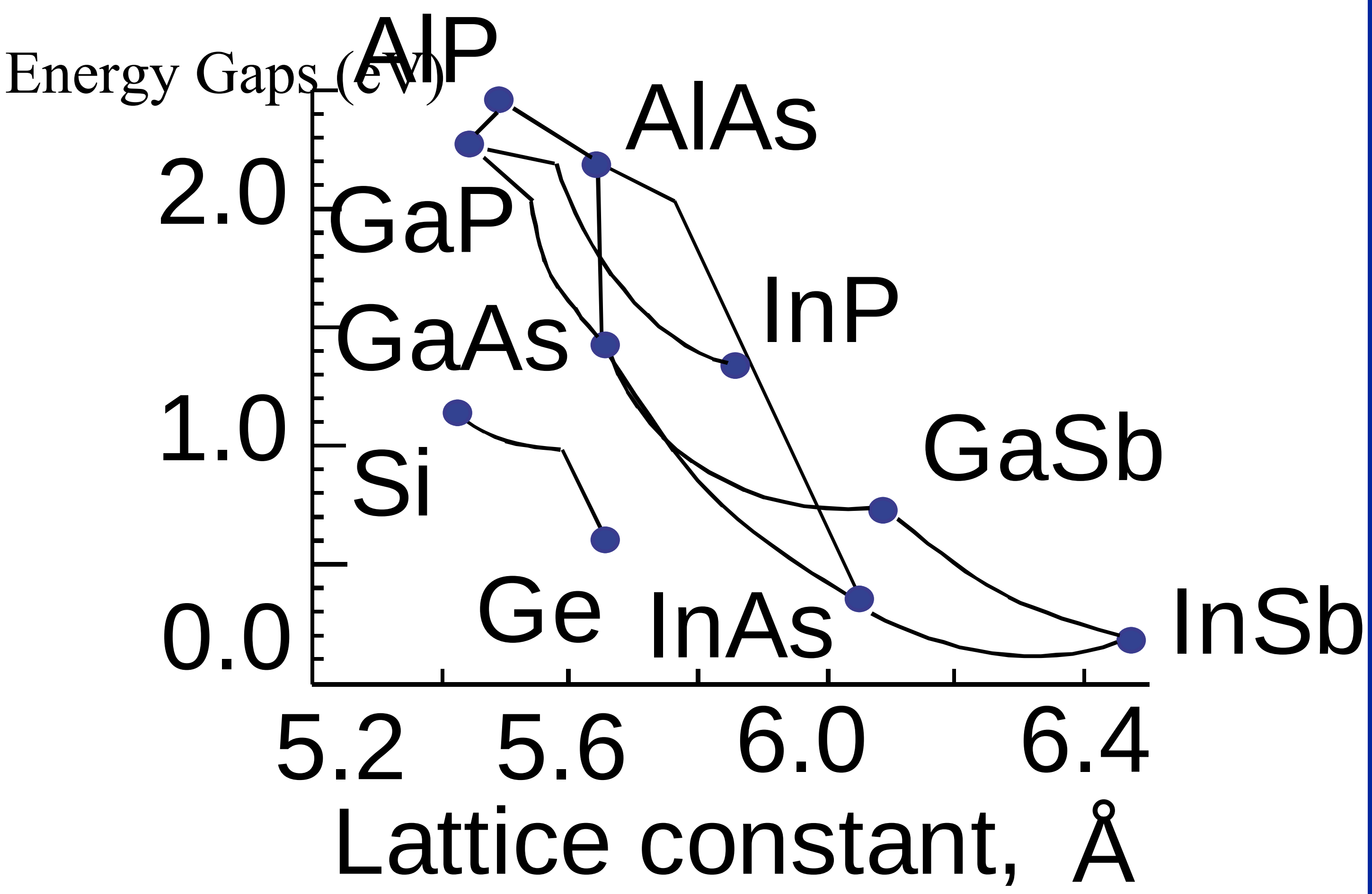
Band diagram basics
Momentum Space



Band diagram basics
Band bending



Energy gaps and lattice constants



Popular Elementary Semiconductors

Si	1.12 eV
Ge	0.661 eV
C (diamond)	5.46 eV
amorphous Si	1.71 eV

See Handbook Series on Semiconductor Parameters, vol. II,
M. Levinshtein, S. Rumyantsev, M. Shur, editors, World Scientific, 1998

Combining elementary semiconductors SiGe SiC SiGeC

Si versus Compounds

Silicon is so great! Why do we need anything else?

Oh, yes, we do, please, please let me explain

Semiconductor industry

University researcher

Reading Assignments

- Reading assignment: Chapters 1, 2, 3

- Review questions

1. What is the de Broglie wavelength of a particle with energy 0.1 eV in a with effective mass of 10^{-31} kg?

Solution

$$\lambda = \frac{2\pi}{k} = \frac{2\pi\hbar}{\sqrt{2m^*E}} = \frac{2\pi \times 1.054 \times 10^{-34}}{\sqrt{2 \times 10^{-31} \times 0.1 \times 1.602 \times 10^{-19}}} = 1.17 \times 10^{-8}(m)$$

More questions

- What is a wave function?
- What is the relationship between photon's momentum and wave vector?
- **4.** What is the relationship between photon's momentum and wavelength?

$p = \hbar k$

More answers

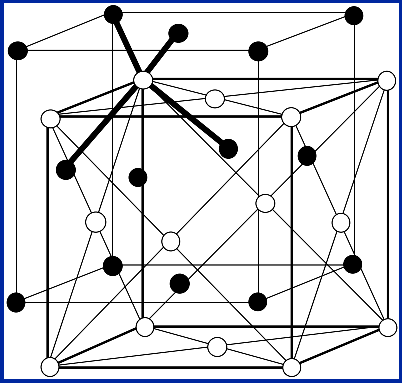
The wave function, Φ(*x*,*y*,*z*,*t*), is an amplitude of the probability density of finding the particle in a given point of space at a given time so that the probability, *P*, of finding a particle in an incremental volume d*x*d*y*d*z* is equal to $|\Phi(x,y,z,t)|^2 dxdydz$.

$$p = \hbar k$$

$$p = \hbar k = \frac{2\pi\hbar}{\lambda}$$

Another Question

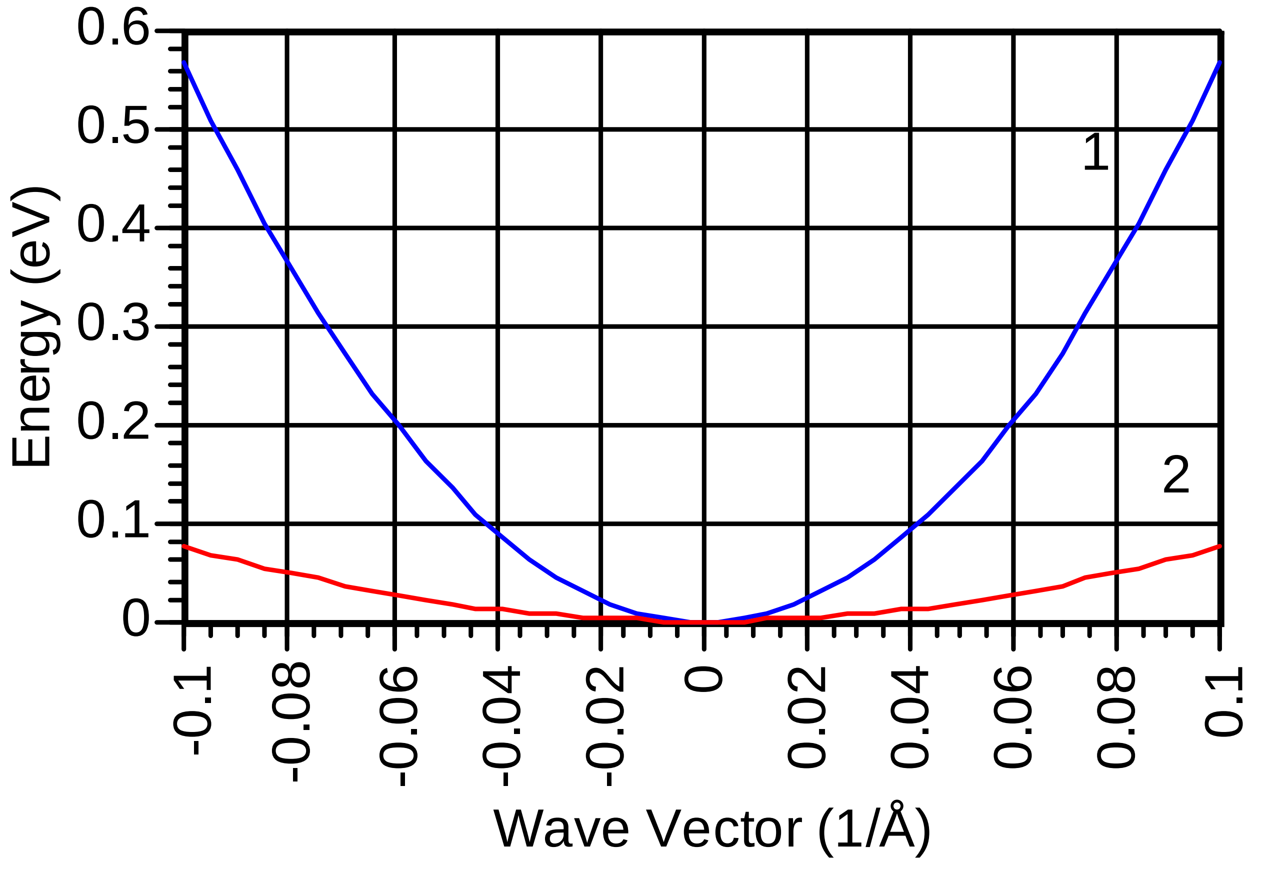
- The crystal structure of a compound semiconductor AB shown in Fig. R3.1 consists of atoms A and B with atomic radii of 1.26 Å and 1.18 Å.
- What is the lattice constant?



Answer

$$a = r_d \frac{4}{\sqrt{3}} = 2.44 \frac{4}{\sqrt{3}} = 5.64\,\mathring{A}$$

What are the effective mass for semiconductors 1 and 2 (in units of the free electron mass)?



Answer

$$E = \frac{\hbar^2 k^2}{2m_e} \quad \frac{m_e}{m_o} = \frac{\hbar^2 k^2}{2m_o qE(eV)}$$

$$\frac{m_{e1}}{m_o} = \frac{\left(1.055\times10^{-34}\right)^2\left(0.1\times10^{10}\right)^2}{2\times9.11\times10^{-31}\times1.602\times10^{-19}\times0.57} = 0.067$$

$$\frac{m_{e2}}{m_o} = \frac{\left(1.055\times10^{-34}\right)^2\left(0.1\times10^{10}\right)^2}{2\times9.11\times10^{-31}\times1.602\times10^{-19}\times0.08} = 0.477$$

Lecture 2

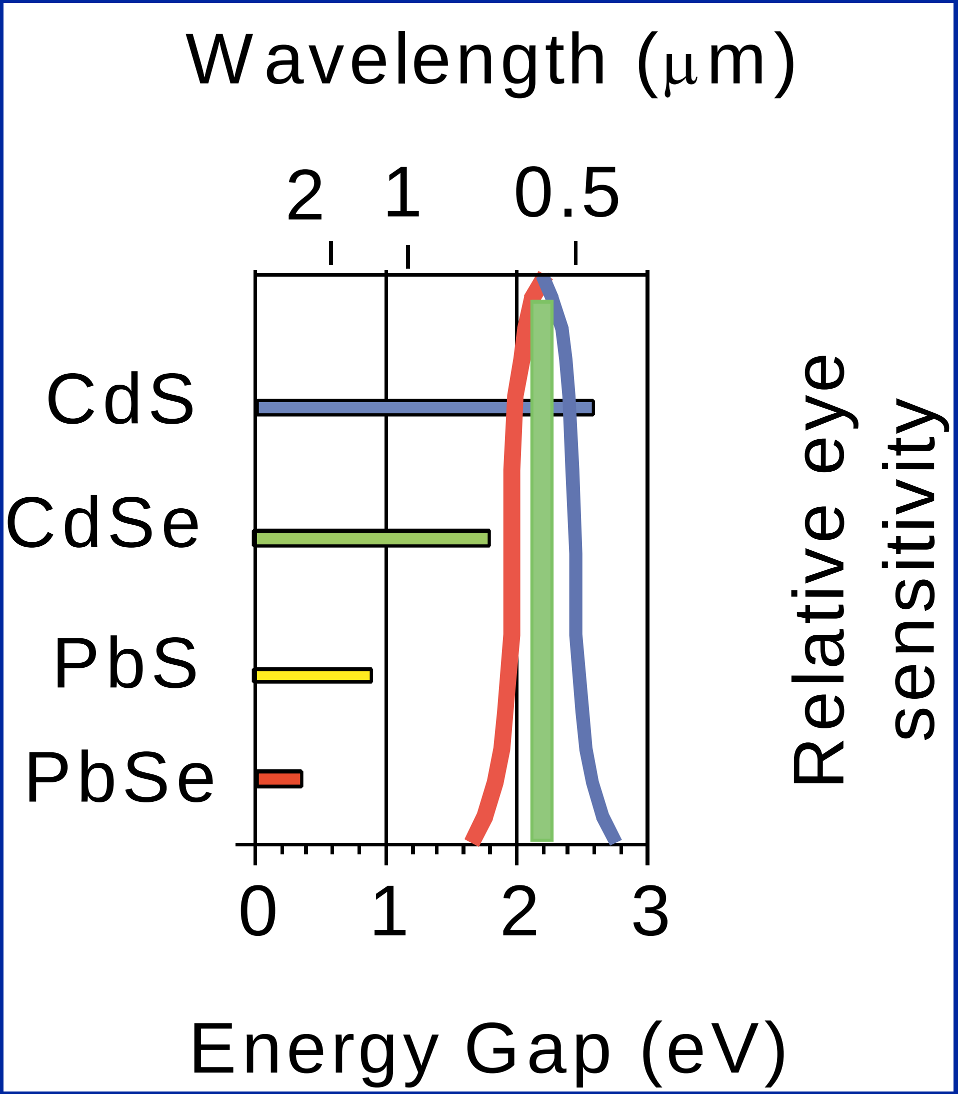
Popular Binary Semiconductors

GaAs	1.41 eV
GaP	2.26 eV
GaSb	0.661 eV
InAs	0.354 eV
InP	1.344 eV
InSb	0.17 eV
SiGe	0.661-1.12 eV
SiC	
GaN/AlN/InN	

See Handbook Series on Semiconductor Parameters, vol. II,
M. Levinshtein, S. Rumyantsev, M. Shur, editors, World Scientific, 1998

CdS, CdSe, PbS, PbSe

- Cover visible range
- Can form heterojunctions
- Could be deposited as thin films on non-conventional (flexible) substrates including textiles
- CdS films on viewfoils have nanocrystalline structure



Wide Band Gap Semiconductors

GaN	3.4 eV
SiC (6H)	2.9 eV
SiC (4H)	3.2 eV
SiC (3C)	2.2 eV
SiC (2R)	
InN	0.8 eV
AlN	6.1 eV

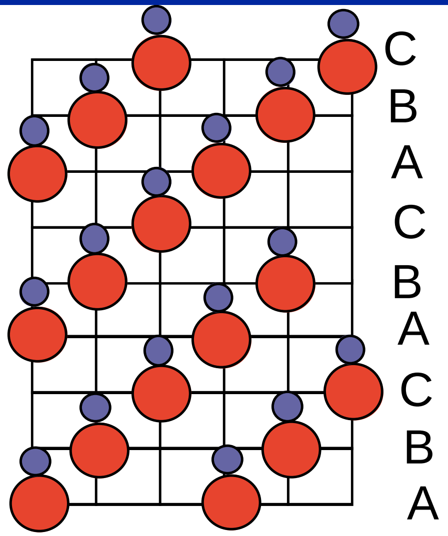
SiC – one of the first semiconductor materials to be discovered

- In 1907, Round observed electroluminescence in silicon carbide, (*Electrical World*, Vol. 19, p. 309, 1907)
- In 1955, Lely developed a new technique of crystal growth for SiC (Lely method)

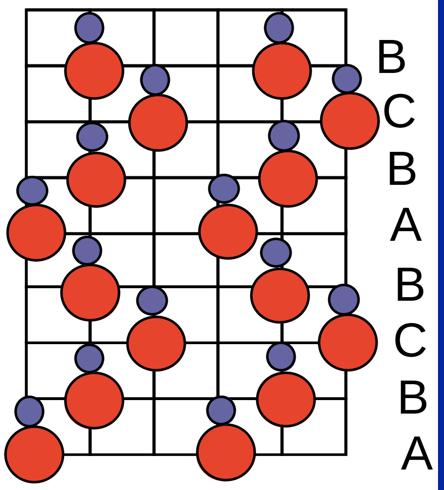
Properties of SiC

- More than 170 different polytypes
- Depending on the polytype crystal structure, the energy gap of silicon carbide varies from 2.2 to 3.3 eV.
- Drift velocity, v_s, of 2×10^7 cm/s
- Breakdown field 2,500 to 5,000 kV/cm (compared to 300 kV/cm for silicon)
- Thermal conductivity up to 4.9 W/cm°C

3C-SiC and 4H-SiC



Cubic polytype
(3C-SiC)



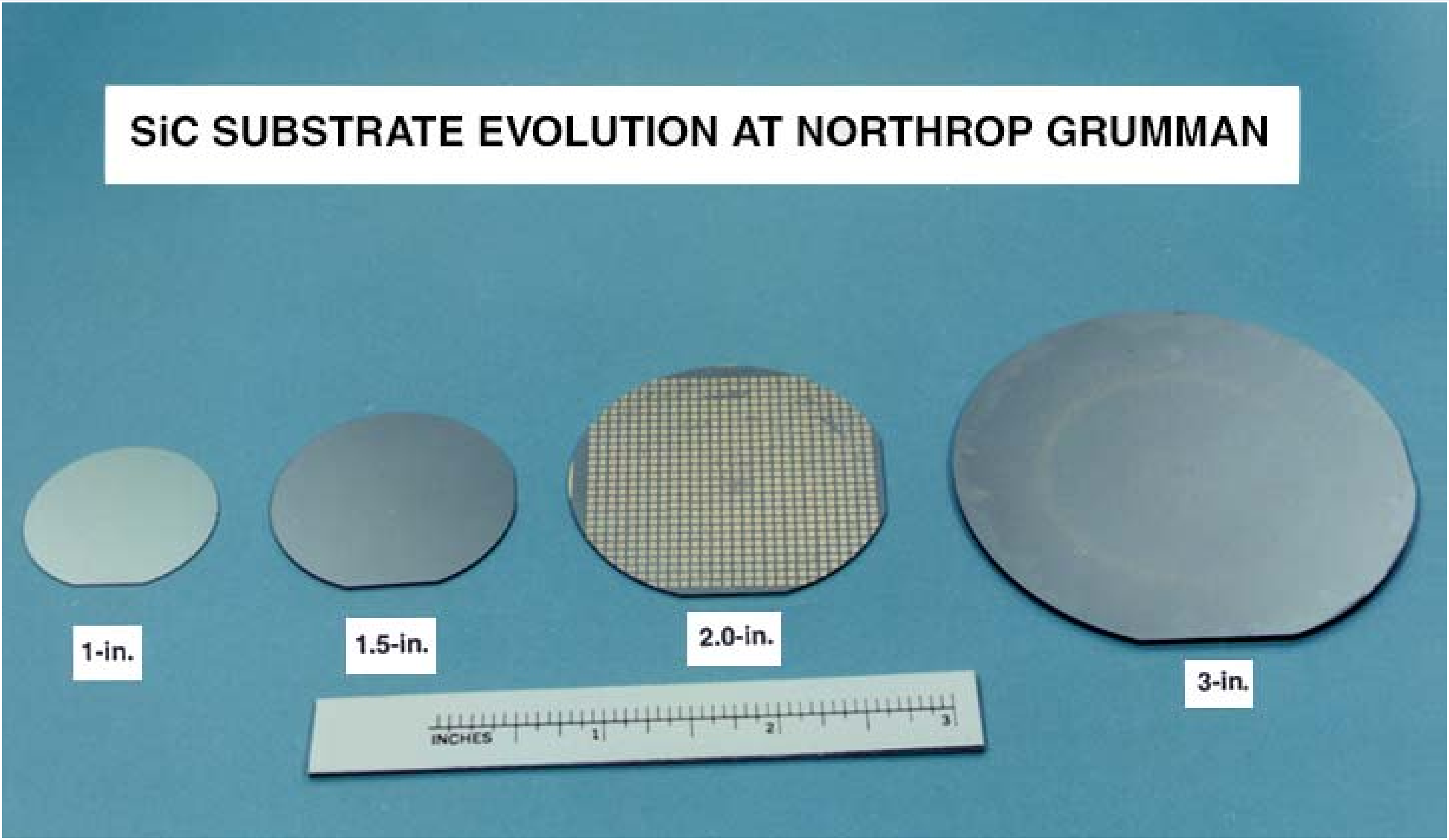
Polytype 4H-SiC
Half sites have
cubic bonding
Half sites have
hexagonal bondibng

- 6H-SiC
  - ABCACBABCA
- 2H-SiC (wurtzite)
  - ABABABABAB

4H-SiC versus 6H-Sic

- 4H-SiC -electron mobility is twice of that for 6H-SiC perpendicular to c-axis
- 4H - SiC -electron mobility is 10 times of that for 6H-SiC perpendicular to c-axis (4H - SiC mobility 800 cm^2/V-s)
- 4H - SiC hole mobility is 30% higher
- For **ionization coefficients of 4H-SiC** see A. O. Konstantinov, Q. Wahab, N. Nordell and U. Lindefelt, Abstracts of International Conference on Silicon Carbide, III-nitride and Related Materials- 1997, August 31 - September 5, 1997 Stockholm, Sweden, Th2b-1, p. 504, (1997)and **Applied Physics Letters -- July 7, 1997 -- Volume 71, Issue 1, pp. 90-92** **(**A hole to electron ionization coefficient ratio of up to 50 was reported)

SiC Wafer Scale-up at Northrop



NORTHROP GRUMMAN
Science & Technology Center

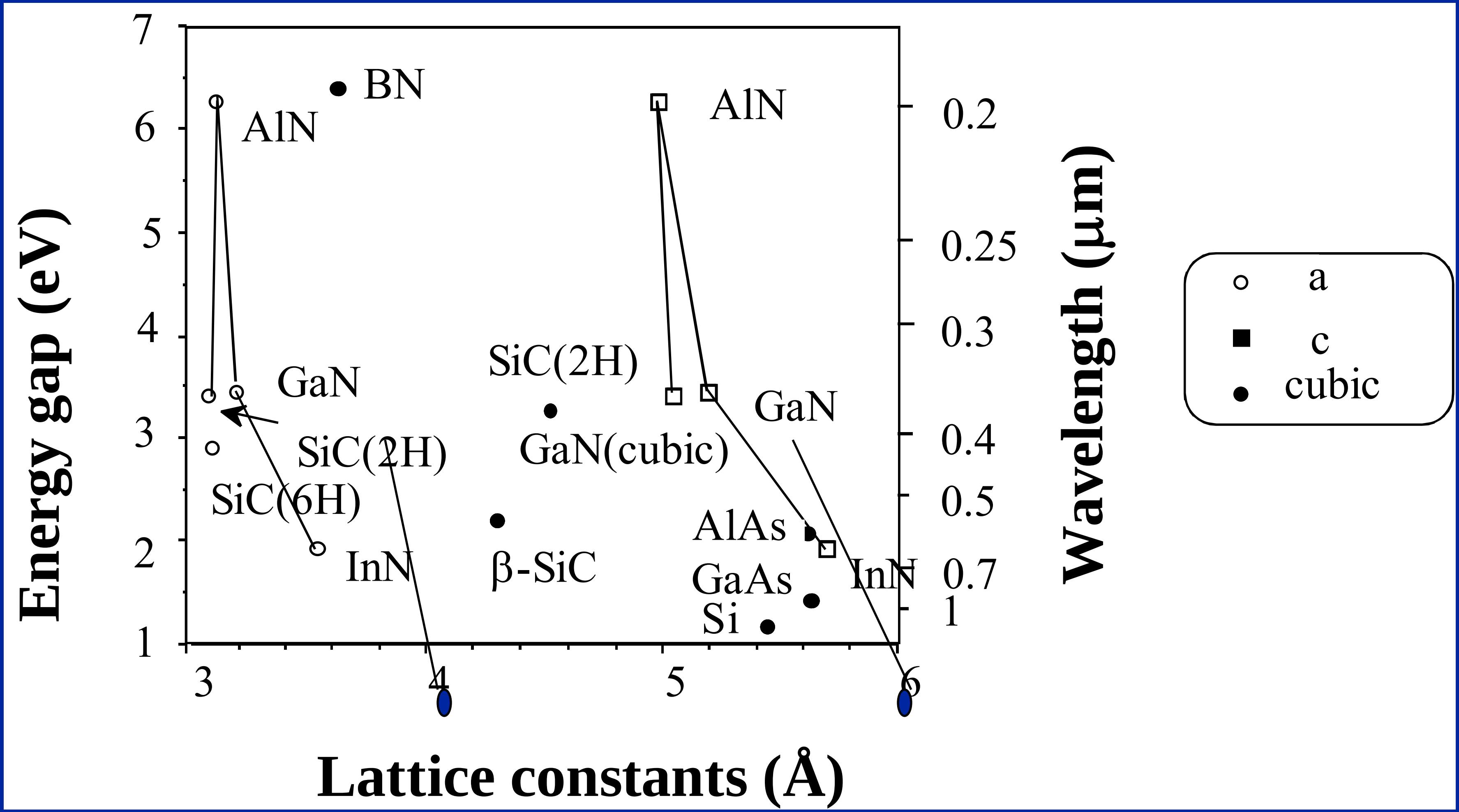
ESSD

Courtesy of Chris Clarke

Toward 4 inch SiC

From www.acq.osd.mil/ott/dpatitle3//highlights.htm

Wide band materials



Basic parameters of InN, GaN, and AlN at 300 K

Parameter	Units	GaN	AlN	InN
Lattice constant, *c*	Å	5.186	4.982	5.693
Lattice constant, *a*	Å	3.189	3.112	3.533
Band gap energy, E_g	eV	3.339[a]	6.2	~~1.97~~ 0.65
Effective electron mass, m_e	m_0	0.19[b] ($\parallel$) 0.17[b] ($\perp$)	0.33[c] ($\parallel$) 0.25[c] ($\perp$)	0.11[b] ($\parallel$) 0.10[b] ($\perp$)
Effective heavy hole mass, m_{hh}	m_0	1.76[c] ($\parallel$) 1.61[c] ($\perp$)	3.53[c] ($\parallel$) 10.42[c] ($\perp$)	1.56[b] ($\parallel$) 1.68[b] ($\perp$)
Effective light hole mass, m_{lh}	m_0	1.76[c] ($\parallel$) 0.14[c] ($\perp$)	3.53[c] ($\parallel$) 0.24[c] ($\perp$)	1.56[b] ($\parallel$) 0.11[b] ($\perp$)
Piezoelectric constant, e_{31}	C/m^2	-0.33	-0.48	-0.57
Piezoelectric constant, e_{33}	C/m^2	0.65	1.55	0.97
Spontaneous polarization, $P_{\parallel}$ [d]	C/m^2	-0.029	-0.081	-0.032
Radiative recombination coefficient[e]	cm^3/s	4.7×10^{-11}	1.8×10^{-11}	5.2×10^{-11}
Refraction index at 555 nm		2.4	2.1	2.8
Absorption coefficient at the photon energy $h\nu \approx E_g$	$10^5\ cm^{-1}$	1	3	0.4

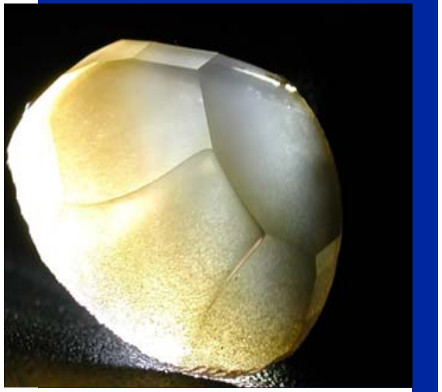
From M. E. Levinshtein, S. L. Rumyantsev, and M. S. Shur, Editors, “Properties of Advanced Semiconductor Materials: GaN, AlN, InN, BN, and SiGe“, John Wiley and Sons, ISBN 0-471-35827-4, New York (2001)

Crystal IS
Innovative Semiconductors

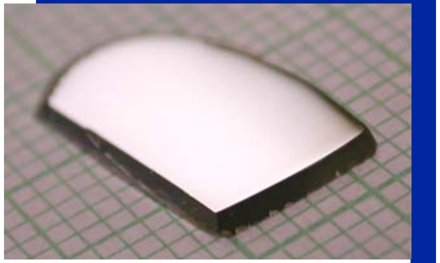
3

Native Aluminum Nitride Substrates

- Key Attributes
  - Long-term lowest cost solution
  - Customer specified orientation (including ***a***, ***b***, and ***c***)
  - Scalable, native-nitride substrates from single crystal boule
  - Lowest dislocation density (<1000 per cm^2; <10 arc-sec *FWHM* triple-axis XRD)
  - High thermal expansion match to III-nitride device structures
  - Isomorphic & lattice-matched to III-nitride device structures
  - High electrical resistivity
  - High thermal conductivity
  - Eliminates need for highly dislocated, low thermal conductivity quasi-buffer layers
- Potential Device Performance Advantages
  - Higher optical & electrical efficiencies
  - Greater gain
  - Higher mobility
  - Longer lifetimes
  - Greater reliability



Single-crystal AlN boule



M-plane substrate

Single crystal AlN substrates recently became available. Fabricated directly from single crystal boules, substrates are available in c-plane, a-plane, and m-plane orientations. CIS believes that AlN will become the long term lowest cost solution for a range of optical and electronic devices.

Narrow Gap Semiconductors

$Hg_xCd_{1-x}Te$	0 eV (at $x = 0.84$ at $T = 0$ K)
grey Sn	0 eV
C (graphite)	0 eV
Certain PbSnTe alloys	

Popular Ternary Compounds

$Al_xGa_{1-x}As$
$In_xGa_{1-x}P$
$In_xGa_{1-x}As$
$In_xGa_{1-x}Sb$
$In_xAs_{1-x}Sb$

SiGeC

$GaAs_xP_{1-x}$

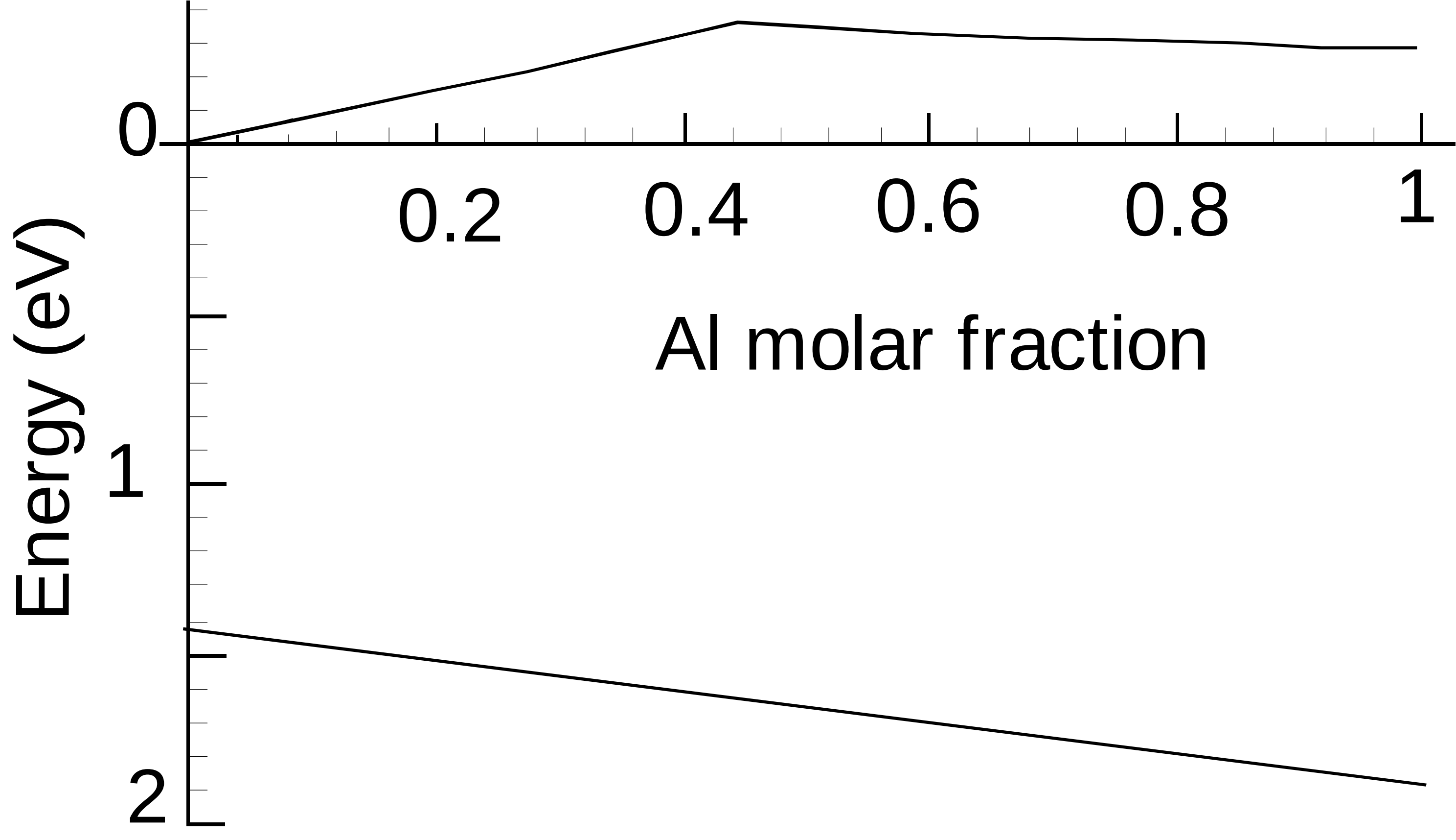
←

See Handbook Series on Semiconductor Parameters, vol. II, M. Levinshtein, S. Rumyantsev, M. Shur, editors, World Scientific, 1998

Popular Quaternary Compounds

$In_xGa_{1-x}\ As_yP_{1-y}$
$In_xGa_{1-x}\ As_yP_{1-y}$

Band Alignment (AlGaAs)



See Handbook Series on Semiconductor Parameters, vol. II,
M. Levinshtein, S. Rumyantsev, M. Shur, editors, World Scientific, 1998

Analytical dependencies

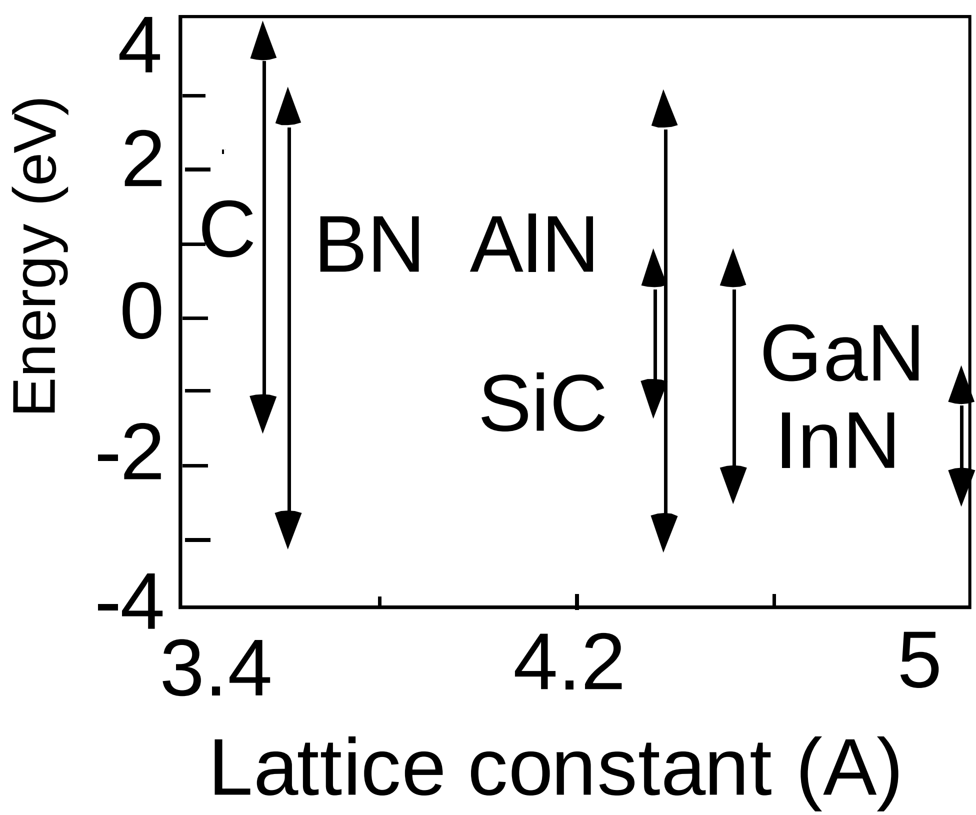
$\Delta E_c = 0.79\ x$ (eV) $x < 0.45$

$\Delta E_c = 0.475 - 0.335\ x + 0.143\ x\text{^}2$ (eV) $x > 0.45$

$\Delta E_v = -\ 0.46\ x$ (eV)

for $Al_xGa_{1-x}As/GaAs$

Band Alignment



After M. W. Wang, J. O. McCaldin, J. F. Swenberg, T. C. McGill , R. J. Hauenstein, Schottky-based band lineups for refractory semiconductors,

Appl. Phys. Lett., 66(15), 1974 (1995).

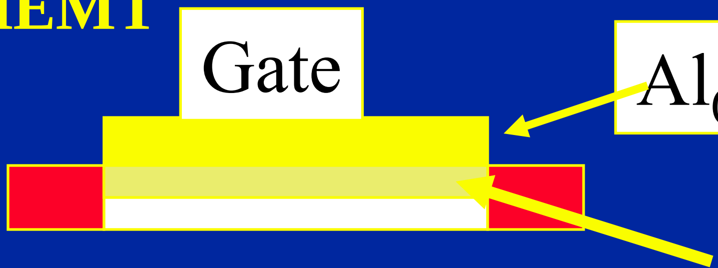
Metals

– Aluminum	3.1 microohm-cm
– Copper	1.7 microohm-cm

Dielectric materials

• SiO_2	Dielectric permittivity	3.9
• Si_3N_4	Dielectric permittivity	7.5
• AF_4 (Low-K)	Dielectric permittivity	2.2
• Air	Dielectric permittivity	1

Example: Gate Leakage



HEMT

Gate

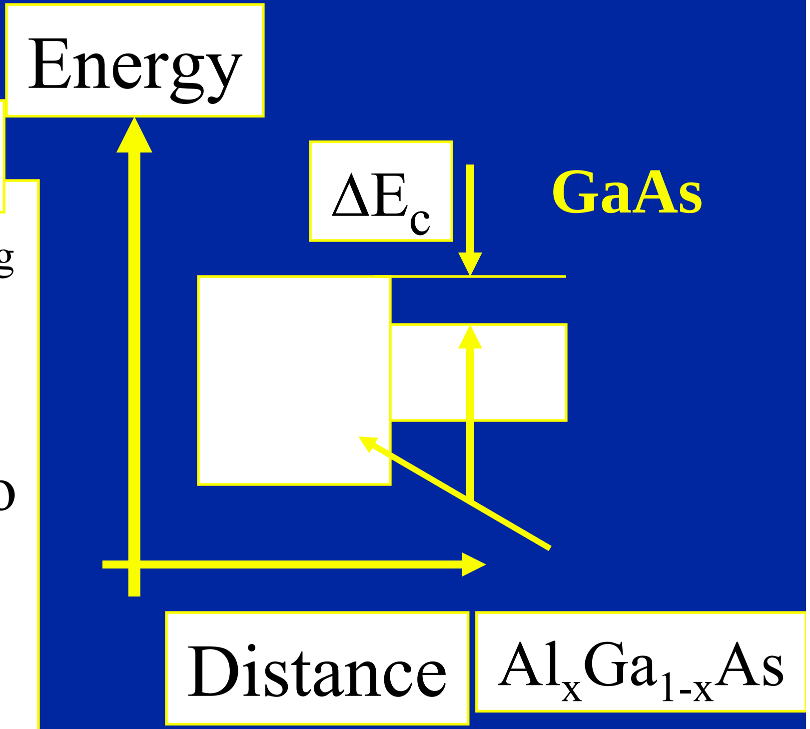
$Al_{0.2}Ga_{0.8}As$ barrier layer

GaAs channel

The leakage gate-to-channel current $I_g = 1\ \mu A$ for T = 300 K.

We would like to decrease to 10 nA.

The leakage is roughly proportional to $\exp(-\Delta E_c/k_BT)$. Is it possible to achieve such a reduction by increasing x?



Energy

ΔE_c

GaAs

Distance

$Al_xGa_{1-x}As$

Solution:

$i_{g1} = A \exp(-\Delta E_{c1}/k_B T)$
$i_{g2} = A \exp(-\Delta E_{c2}/k_B T)$

$i_{g2} / i_{g1} = \exp[(\Delta E_{c1} - \Delta E_{c2})/k_B T]$

Hence,

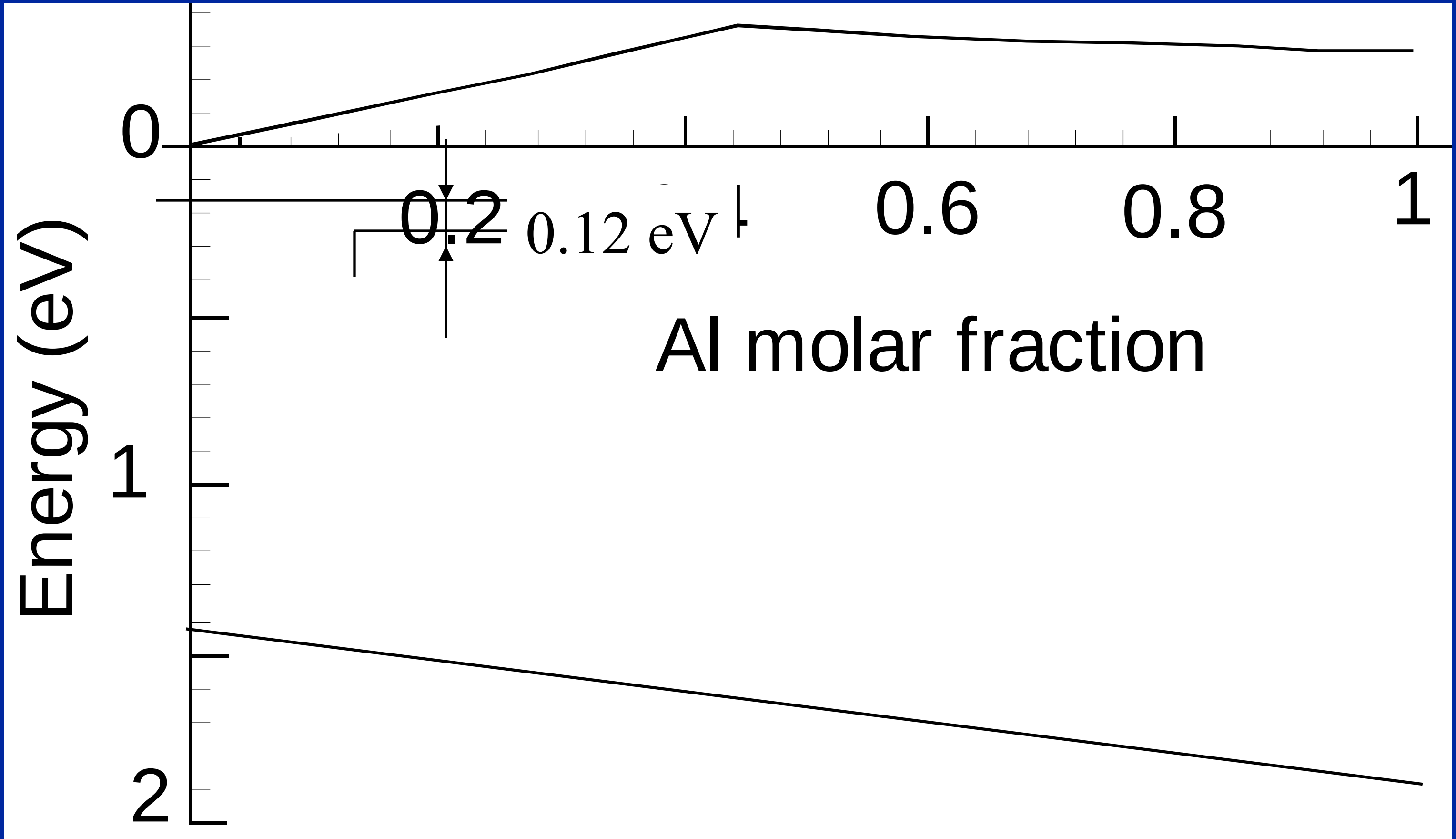
$\Delta E_{c1} - \Delta E_{c2} = k_B T \ln (i_{g2} / i_{g1})$

or, in eV:

$\Delta E_{c1} - \Delta E_{c2} = 0.026 \ln(100) = 0.12$ (eV)

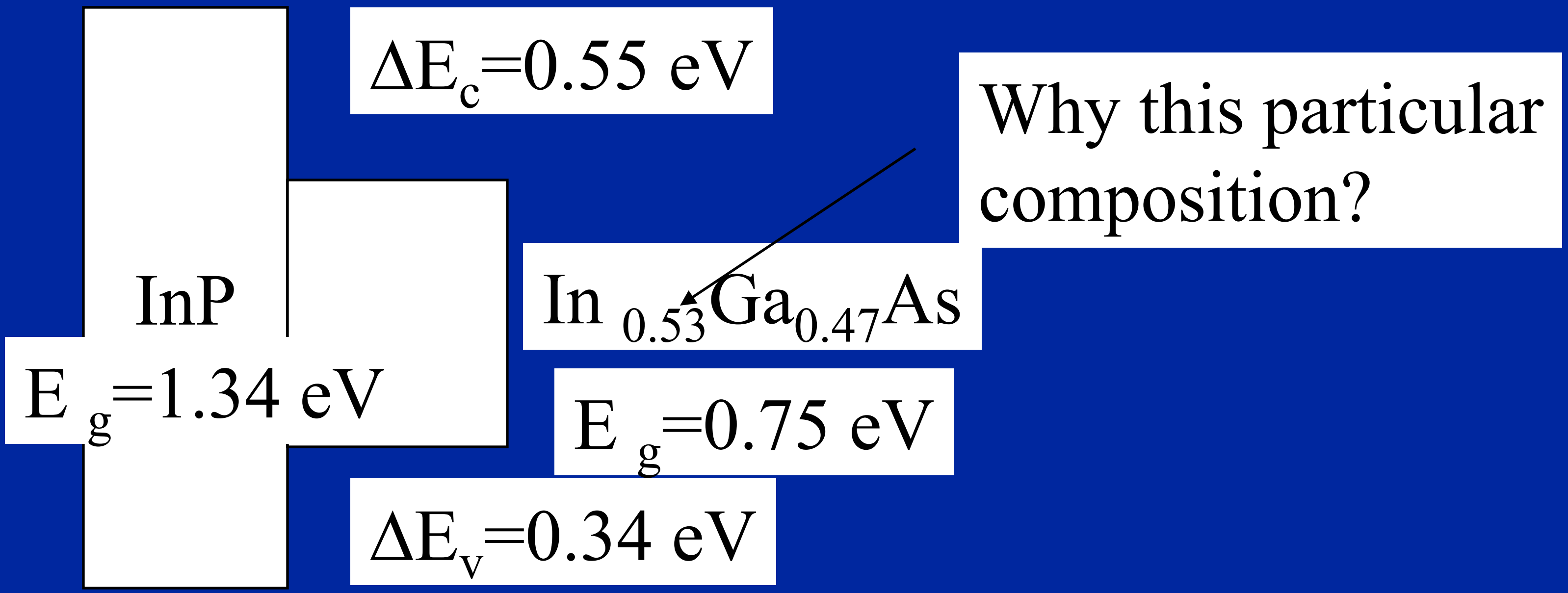
3

Solution (continued)



x = 0.36 or so is required

Example 2. Band Alignment



$\Delta E_c = 0.55$ eV

InP

$E_g = 1.34$ eV

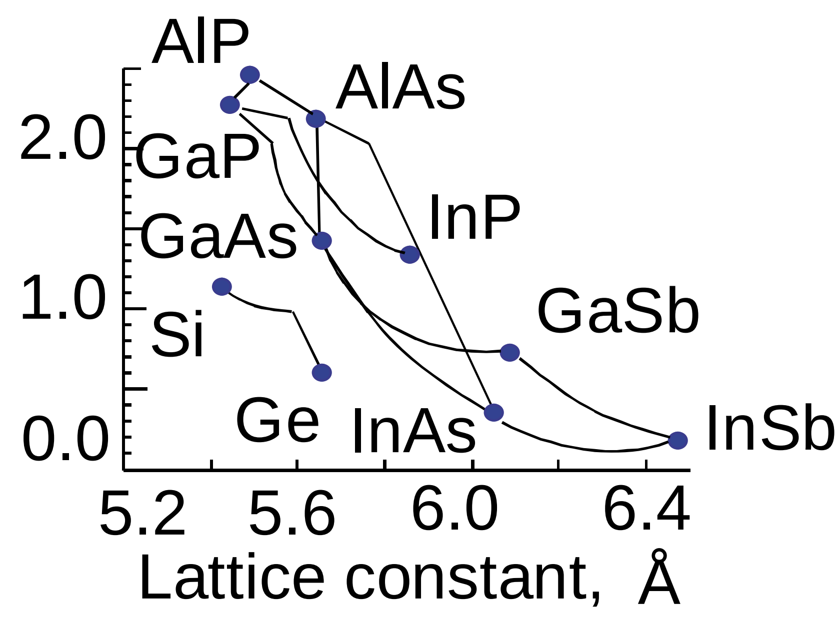
Why this particular composition?

$In_{0.53}Ga_{0.47}As$

$E_g = 0.75$ eV

$\Delta E_v = 0.34$ eV

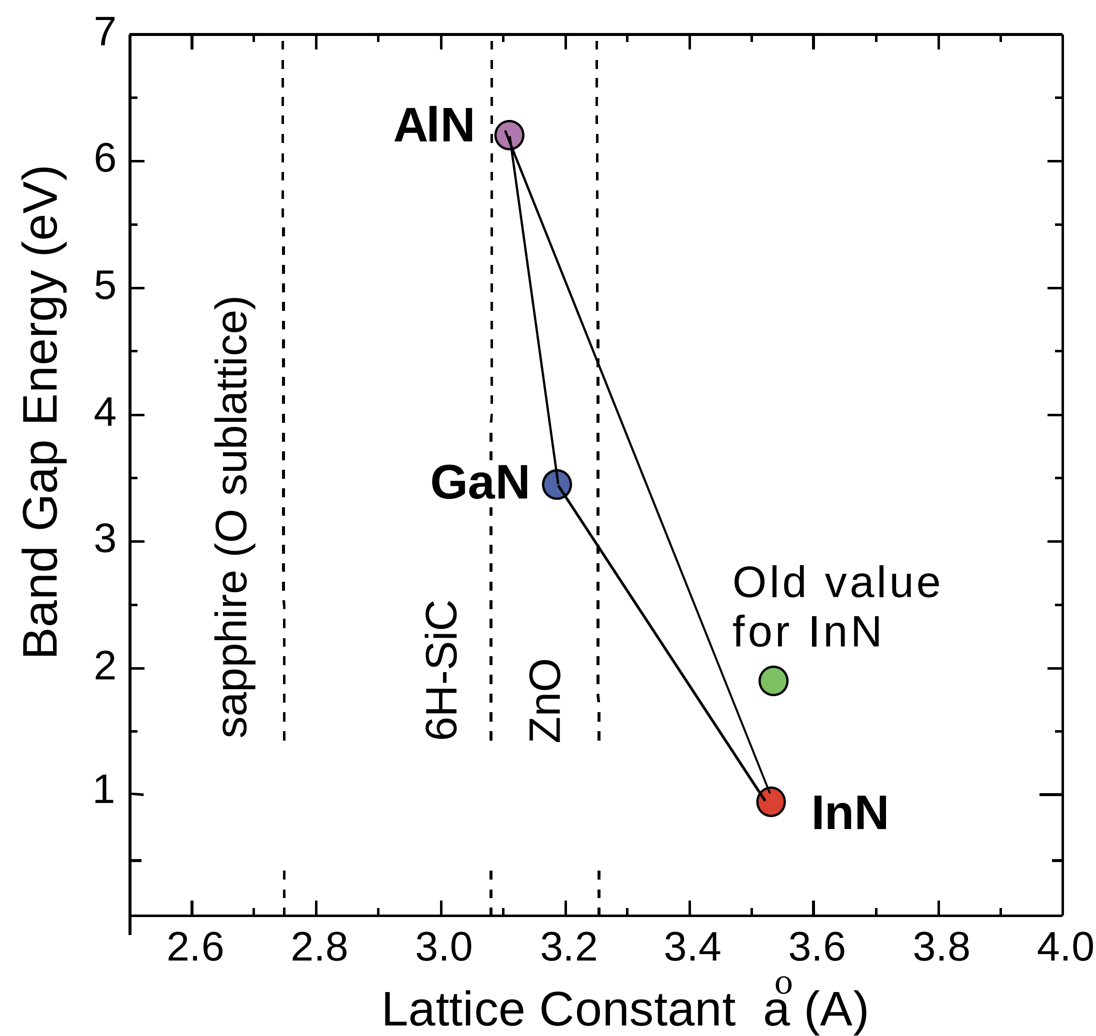
$In_{0.53}Ga_{0.47}As$ Lattice-Matched to InP



At x = 0.53 $In_{0.53}Ga_{0.47}As$ is lattice-matched to InP shurm@rpi.edu

3

AlInGaN Materials System



Before-Pankove_Maruska Era (BPM-Era)

- 1932 – Roosevelt wins Presidential Election. First GaN crystal synthesized W. C. Johnson, J.B. Parsons, and M. C. Crew, J. Phys. Chem. 36, 2651 (1932)
- 1936 – Spanish Civil War starts. First Russian GaN crystal synthesized G. S. Zhdanov and G. V. Lirman. Zh. Exp. Teor. Fiz.6, 1201 (1936)
- 1961 – Yuri Gagarin becomes the first man in space. First p-type GaN A. G. Fischer, Solid-State Electron. 2, 231 (1961)

Pankove-Maruska Era (P-Era)

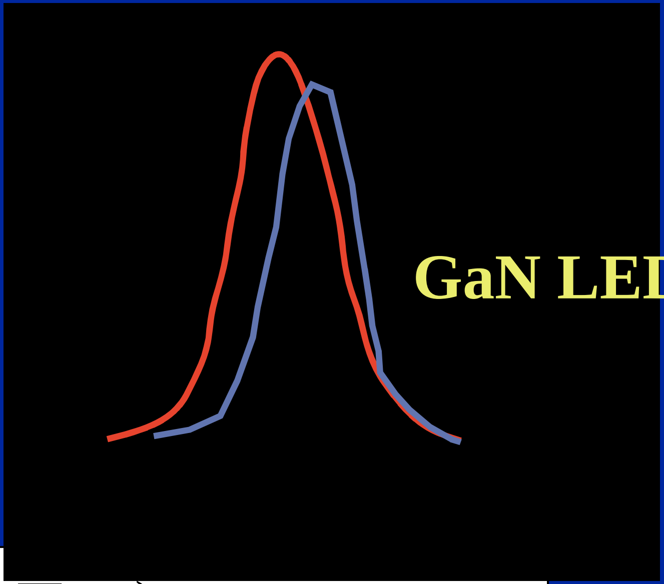
- 1969 – First Moon walk by Armstrong and Aldrin. Another GaN crystal by HVPE H. P. Maruska and J. J. Tietjen, Appl. Phys. Lett. 15, 327 (1969)
- 1969 – Cadaffi comes to power. First monograph on nitrides G. V. Samsonov, Nonmetallic Nitrides, in Russian, Naukova Dumka, Kiev (1969)
- 1971- Bangladesh Independence. First GaN LED J. I. Pankove, E. A. Miller, and J. E. Berkeyheiser, J. Lumin. 4, 63 (1971)

Pankove and Maruska

Pankove-Maruska LED (1971)

Art by J. Pankove

(untitled, Michael Shur’s Collection, the gift from the artist)



After Pankove-Murarka (APM-Era) :

- 1973 First review paper on GaN English translation: . P. Kesamanly, Sov. Phys. Semicond. Vol. 8, No. 2, 147 (1974)

Nitride Advantages for Electronic Devices

Properties

- High mobility
- High saturation velocity
- High sheet carrier concentration
- High breakdown field

→ **High power**

- Decent thermal conductivity
- Growth on SiC substrate

→ **Heat handling capability**

- Chemical inertness
- Good ohmic contacts
- No micropipes

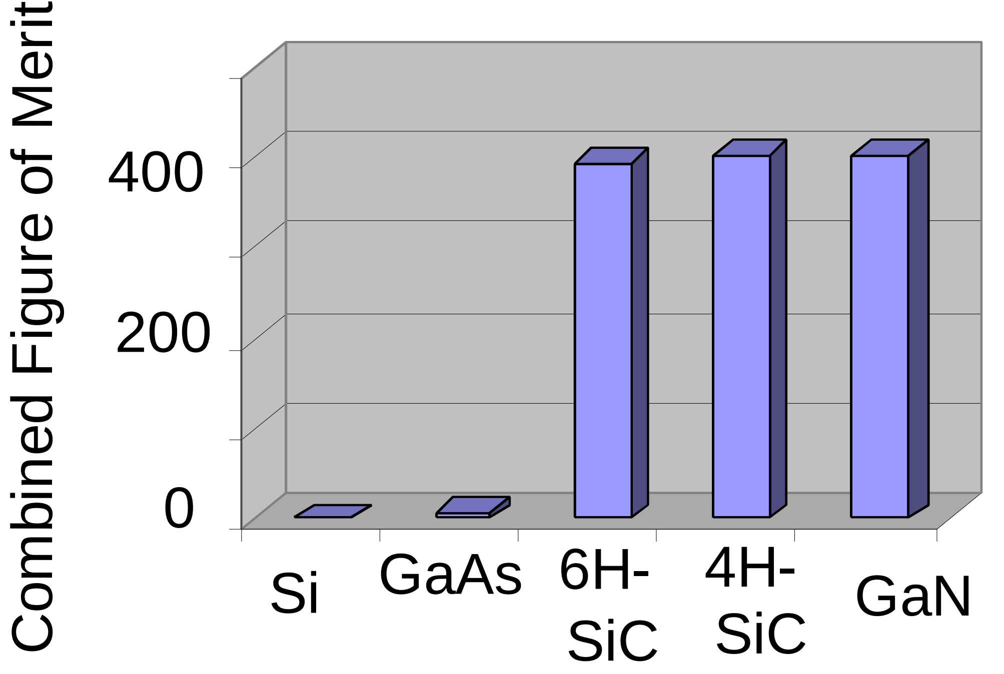
→ **Reliability**

- SiO_2/AlGaN and SiO_2/GaN good quality interfaces

→ **Insulated Gate**

Advantages

Figure of Merit for high frequency/high power



$$CFOM = \frac{\chi \varepsilon_o \mu v_s E_B^2}{\left(\chi \varepsilon_o \mu v_s E_B^2\right)_{silicon}}$$

χ is thermal conductivity

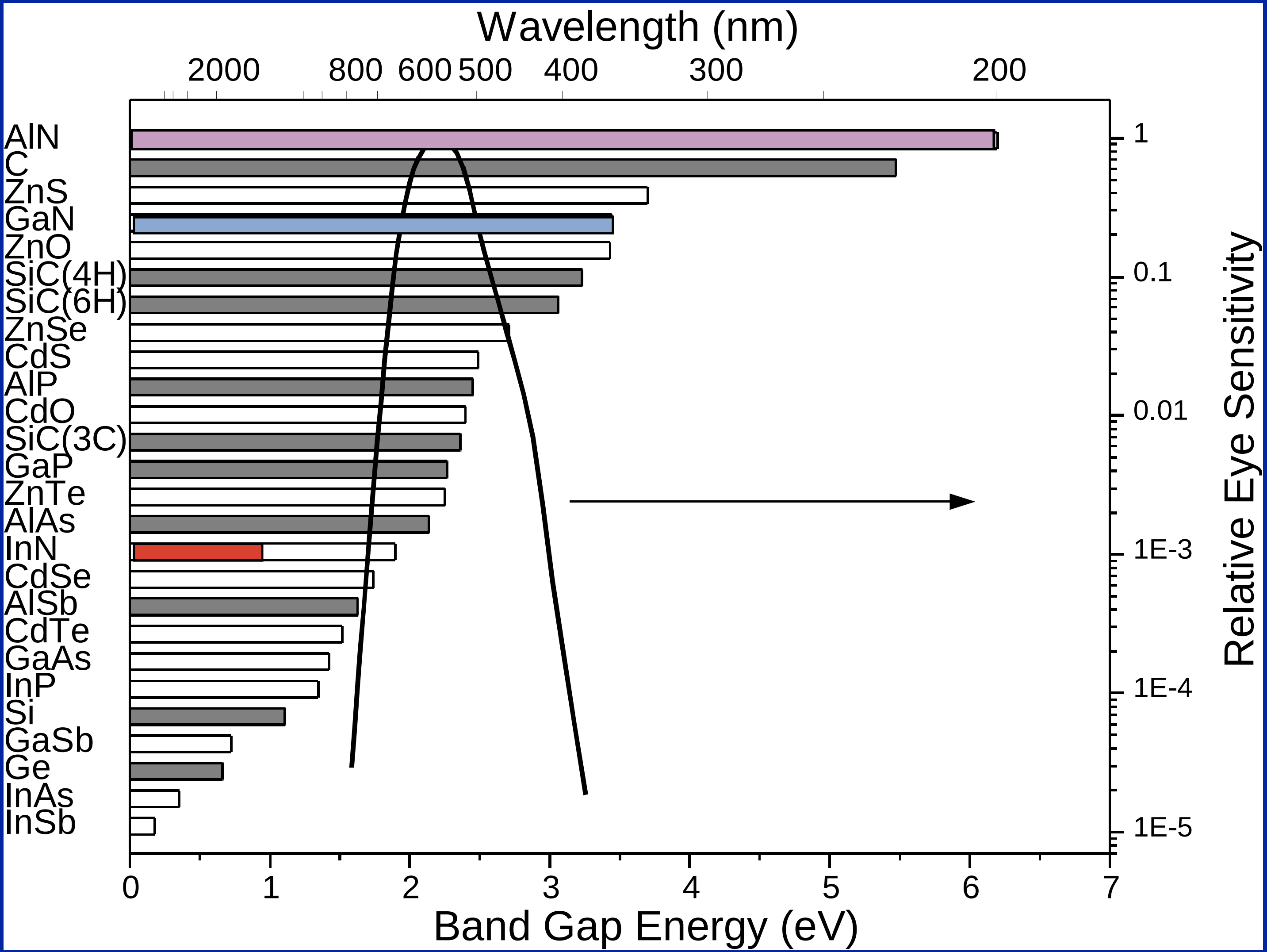
E_B is breakdown field

μ is low field mobility

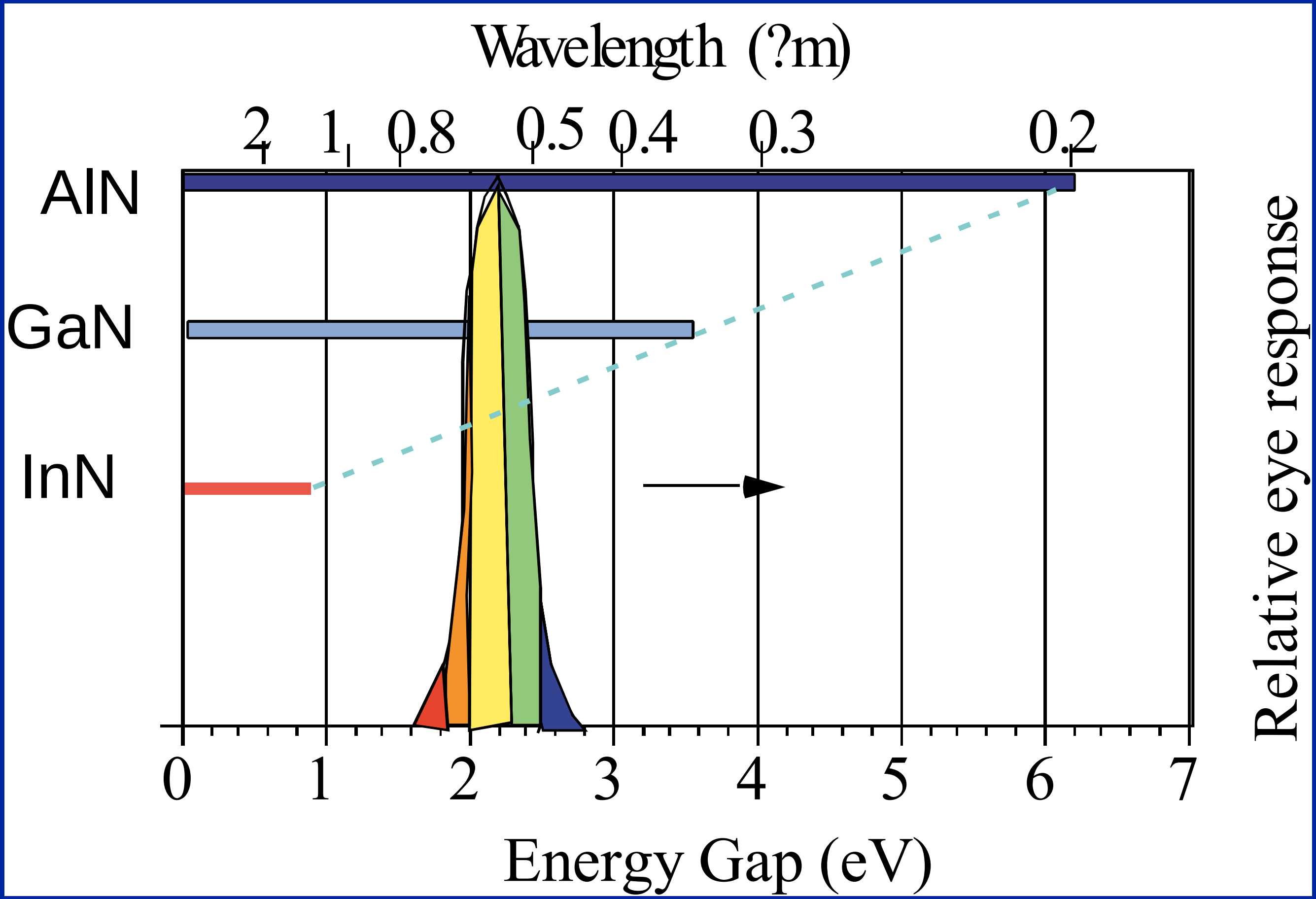
v_s is saturation velocity

ε_o is dielectric constant

SEMICONDUCTOR MATERIALS SYSTEMS FOR LIGHT EMITTERS



Energy gaps of nitrides compared with spectral sensitivity of human eye



Problems to Solve

- Aging
- Substrates
- Current slump
- Cost
- Yield
- Manufacturability