# FoP 3B Part II

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Room 151

## Lecture 1: Band gaps in Semiconductors

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# Course outline

## Semiconductors

**Lectures 1-6**

**Example Class 1,2**

**Weekly Problem Set 1, 2, 3**

## Superconductors

**Lectures 7-9**

**Example Class 3,4**

**Weekly Problem 4**

## Dielectrics

**Lectures 10-12**

**Example Class 5**

**Supplementary Weekly Problems**

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**+ 1 Revision Lecture (May)**

# Suggested Reading

(1) C Kittel, *Introduction to Solid State Physics* (course broadly based on this textbook)
(2) DA Neamen, *An introduction to Semiconductor devices* (Chapters 3,5; easy reading)
(3) JF Annett, *Superconductivity, Superfluids and Condensates* (Chapter 3, 4)
(4) NW Ashcroft and ND Mermin, *Solid State Physics* (slightly more advanced)

Lecture summaries available on Blackboard Ultra

# Aim of today's lecture

Q: How is a semiconductor different from a metal?

A: Band gaps

*Key concepts:*

-Origin of band gaps (review of previous material)
-Example crystal structures of semiconductors
-Direct vs indirect band gaps and Vegard's law
-Effective mass of electrons

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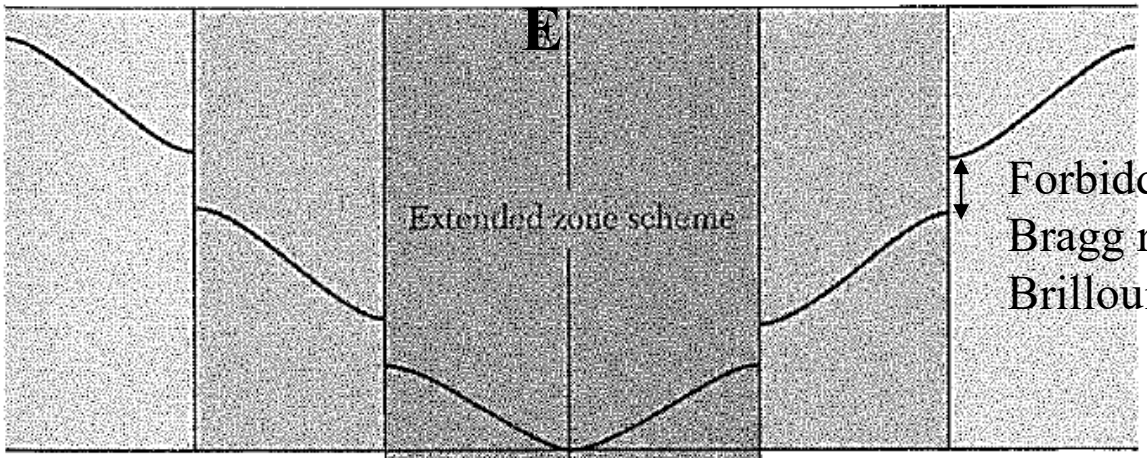
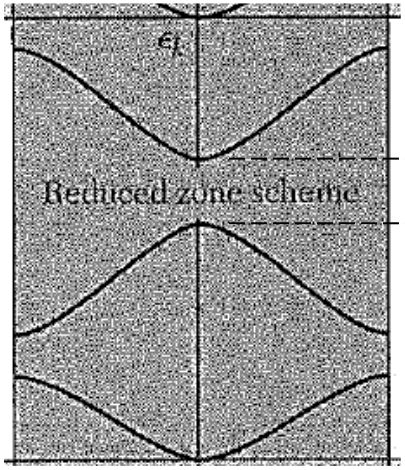
# Origin of band gaps (revision)




Forbidden band due to Bragg reflection at Brillouin zone boundary

Extended zone scheme




Forbidden band

Reduced zone scheme

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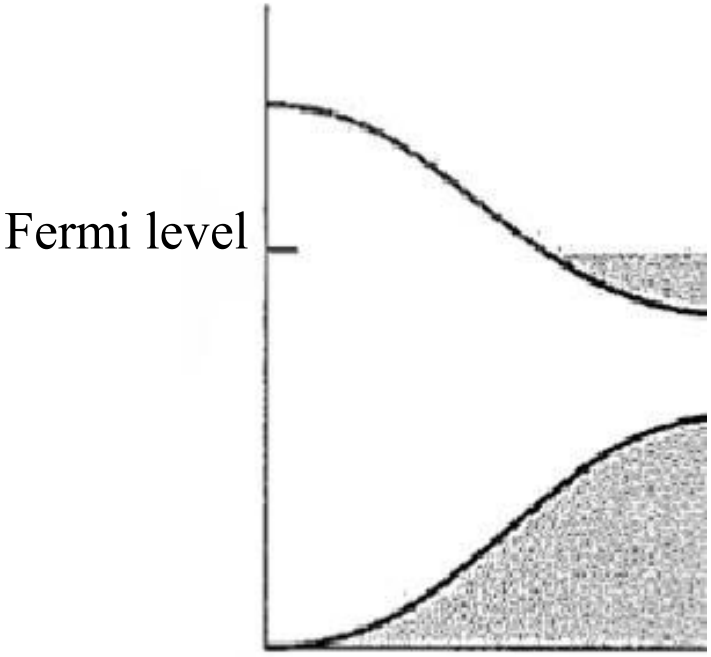
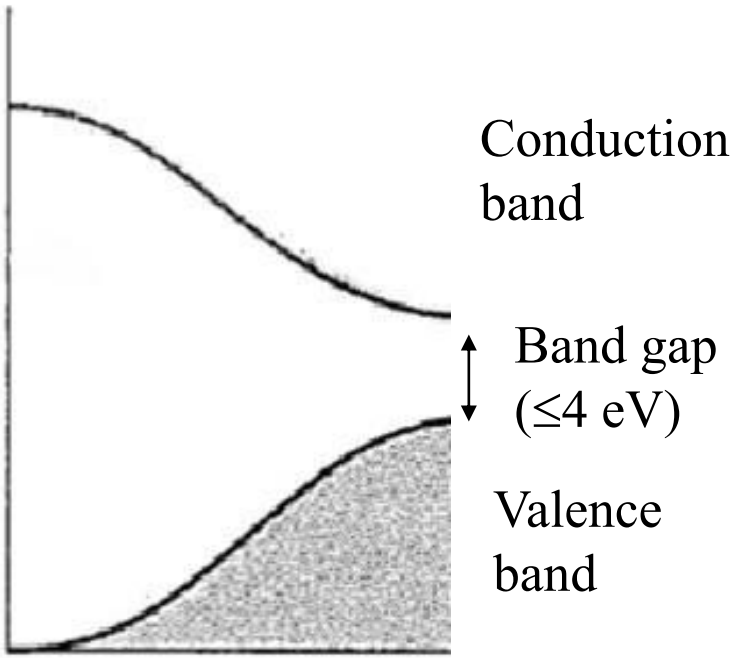
# Metals vs semiconductors




Metal: incompletely filled conduction band




Semiconductor: valence (conduction) band completely full (empty) at 0 K*

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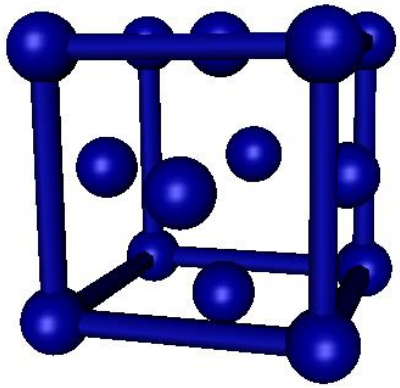
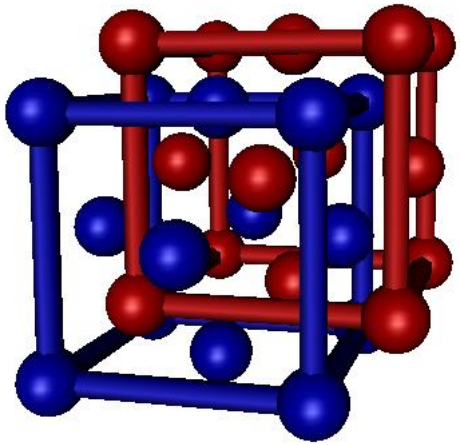
* A primitive cell can have two electronic states within a given band

# Examples of semiconductors (diamond lattice)

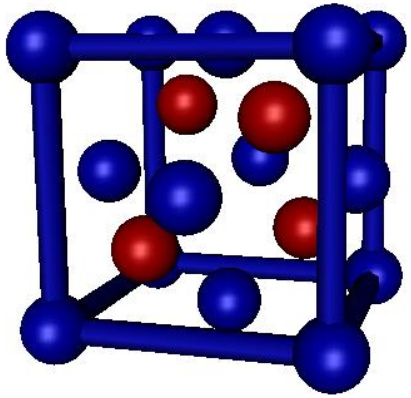
Elemental semiconductors, such as Si = $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^2$.



An fcc lattice



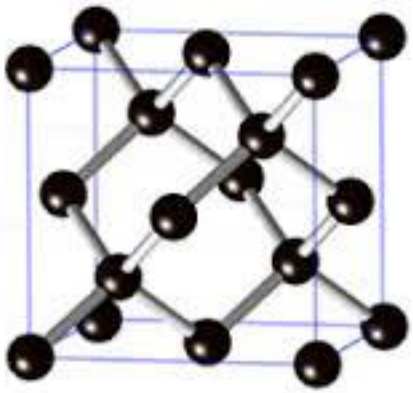
Two fcc lattices shifted by (1/4,1/4,1/4).



Keeping only atoms inside the cubic unit cell

If all atoms are the same:

Each atom has four bonds (Group IV; octet rule).



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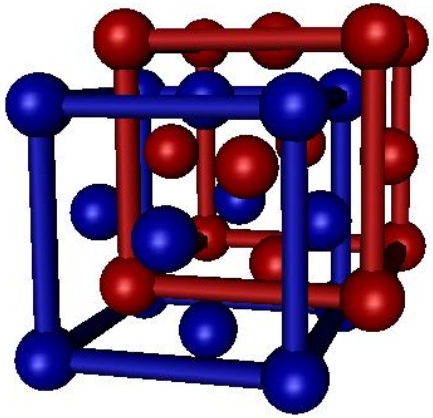
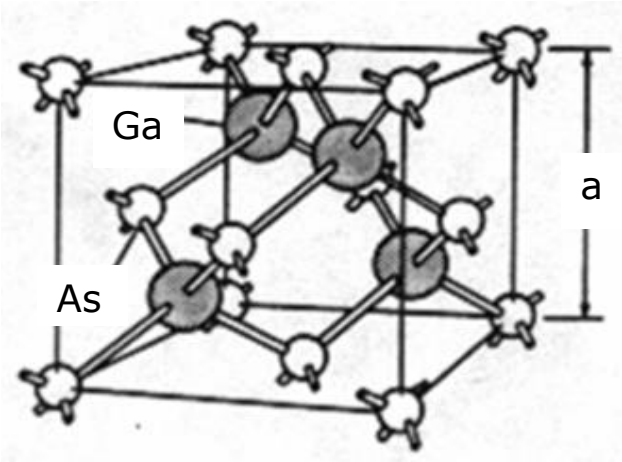
# Compound semiconductors (zinc blende structure)



If there are two atom types

e.g. ZnS, **GaAs**, CdTe

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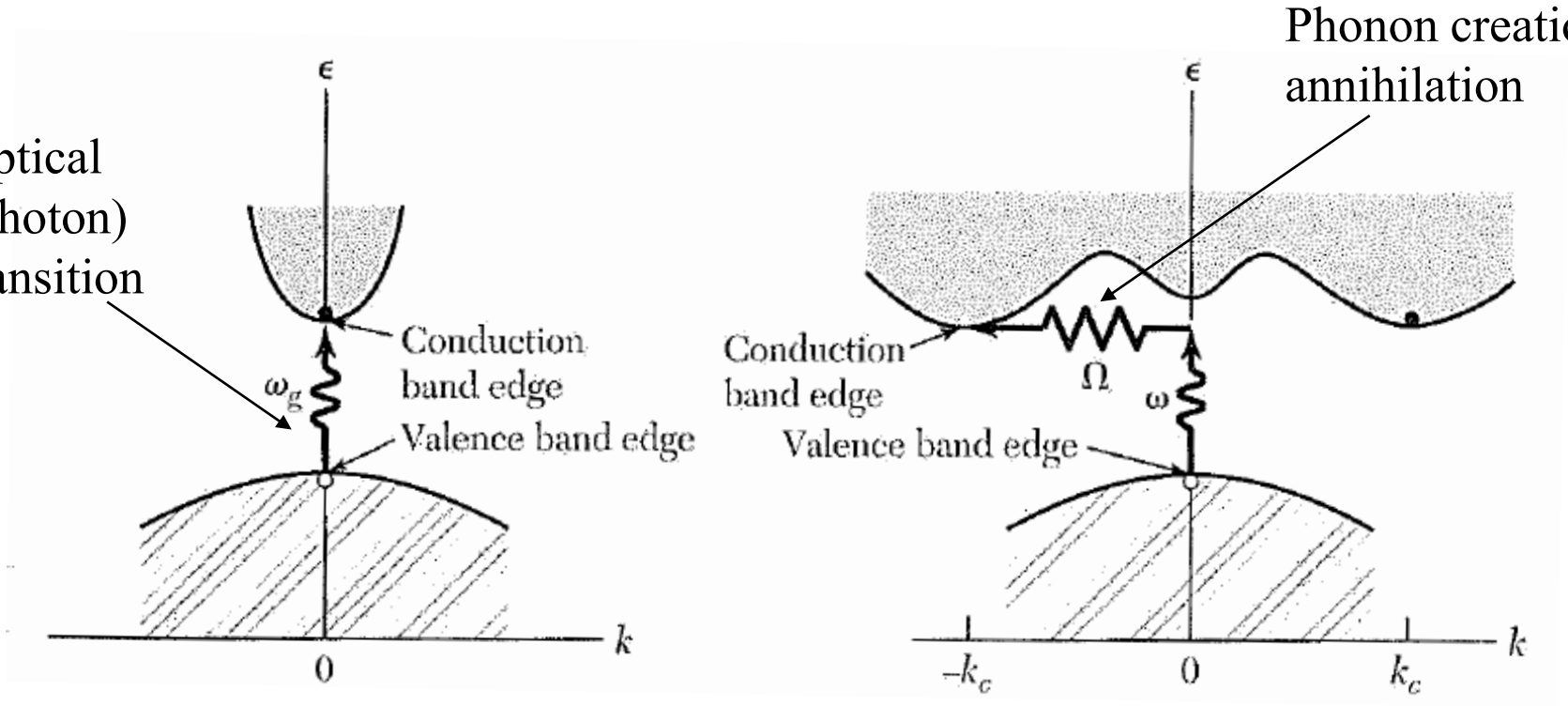
# Direct vs indirect band gaps (photon absorption)

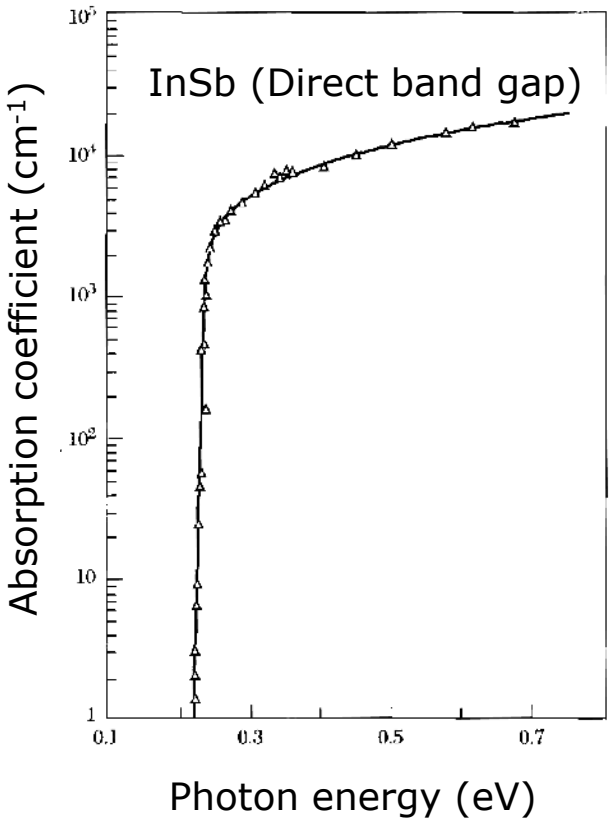


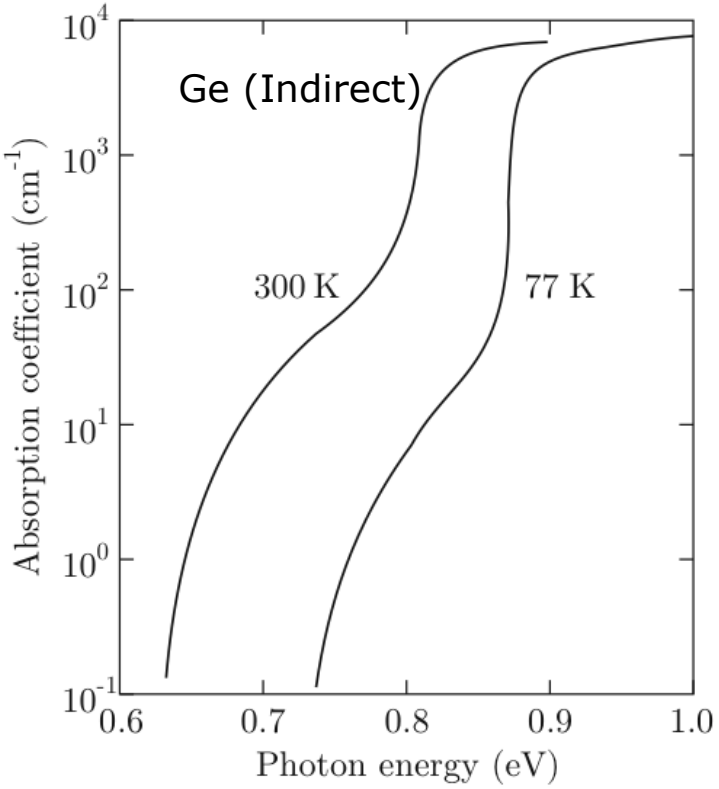

Direct band gap

Indirect band gap

Band gap is the minimum photon energy required to promote an electron into an unoccupied level. Both energy and momentum must be conserved during the transition.

# Band gap measurement (photoabsorption)




NB: Weak absorption onset and strong temperature dependence for indirect band gap (due to phonon mediation)

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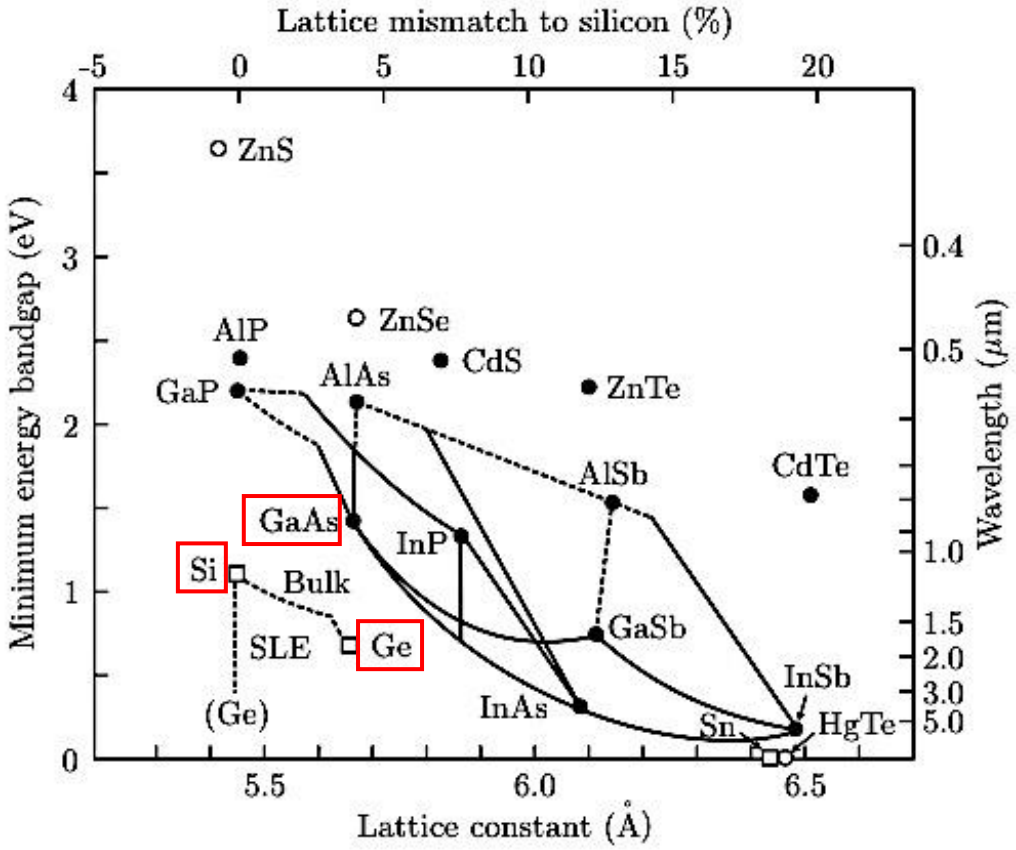
# Band gap variations in alloy semiconductors

For many applications, it is **desirable** to **tune** the value of the band gap.




Solid curves - direct gaps.

Dashed curves - indirect gaps.

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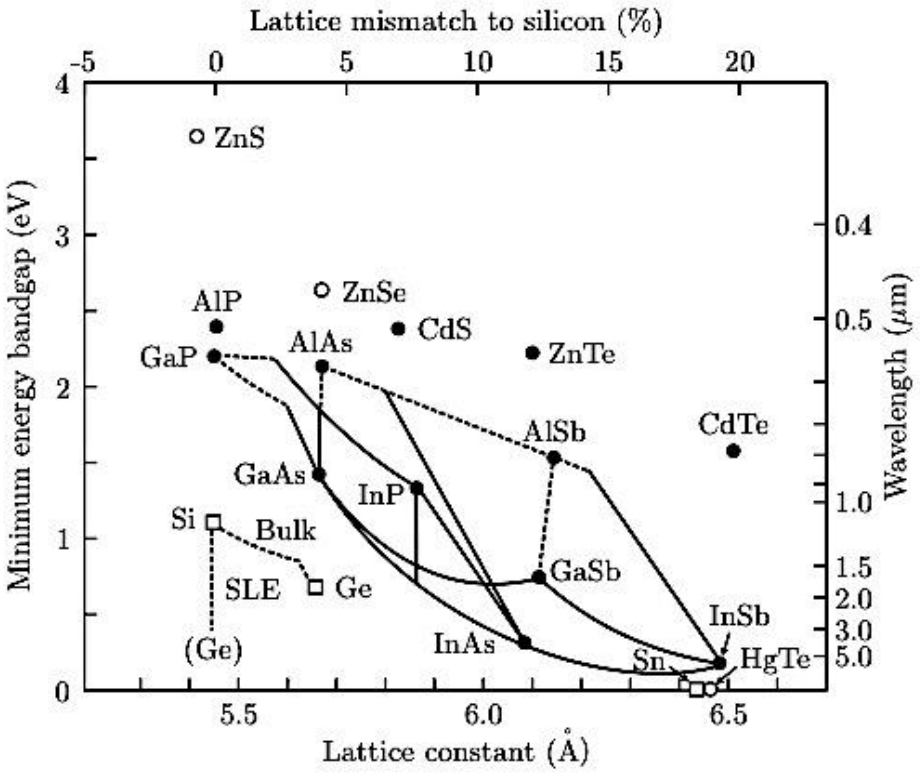
# Vegard's law




For a semiconductor alloy* $A_xB_{1-x}$

**Band gap energy**

$$E_{g,AB} = xE_{g,A} + (1-x)E_{g,B} - bx(1-x)$$

b is called the **Bowing parameter**

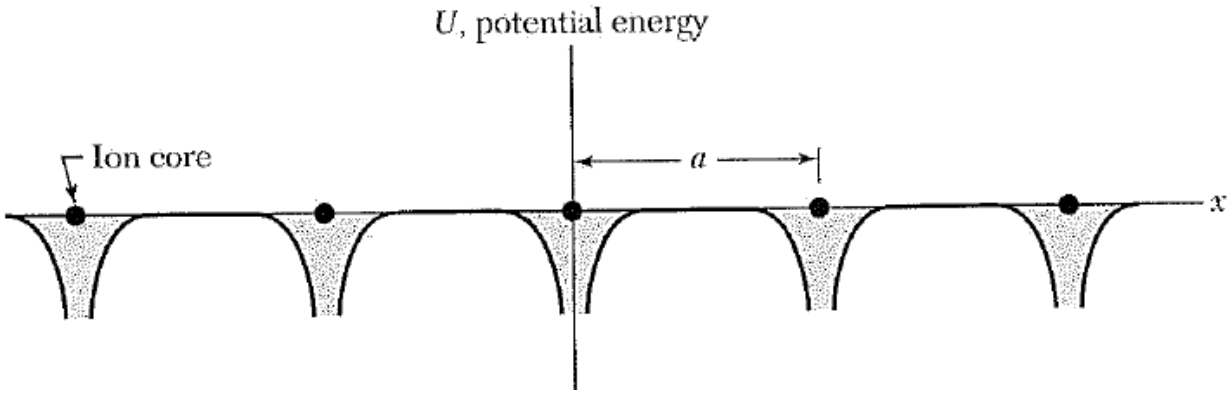
**Lattice Parameter:**

$$a_{AB} = xa_A + (1-x)a_B$$

* A, B can represent elements or compounds (e.g. Si/Ge or GaAs/InAs)

In device applications the semiconductor is typically deposited on a substrate. The lattice parameter of the semiconductor and substrate must be similar to minimise strain.

# ‘Effective’ mass of electrons in a crystal




- Electrons in a crystal are subjected to a periodic potential from the ion-cores.
- The response to an external force $F$ (e.g. electric/magnetic field) is therefore different to an electron in free space.
- Define an effective mass $m^*$, such that $F = m^*a$ is obeyed.

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# Expression for effective mass*

*Key Results:*

$$\mathbf{v} = \frac{d\omega}{dk} = \frac{1}{\hbar}\frac{dE}{dk}$$

(group velocity of Bloch wave)

$$\boxed{\mathbf{F} = \hbar\frac{d\mathbf{k}}{dt}}$$

Substituting in $F = m^*a = m^*(dv/dt)$ gives:

$$\boxed{m^* = \hbar^2 / \frac{d^2E}{dk^2}}$$

For anisotropic crystals (effective mass tensor):

$$\boxed{m_{ij}^* = \hbar^2 / \frac{d^2E}{dk_i dk_j}}$$

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* See supplementary notes for a derivation (non-examinable)