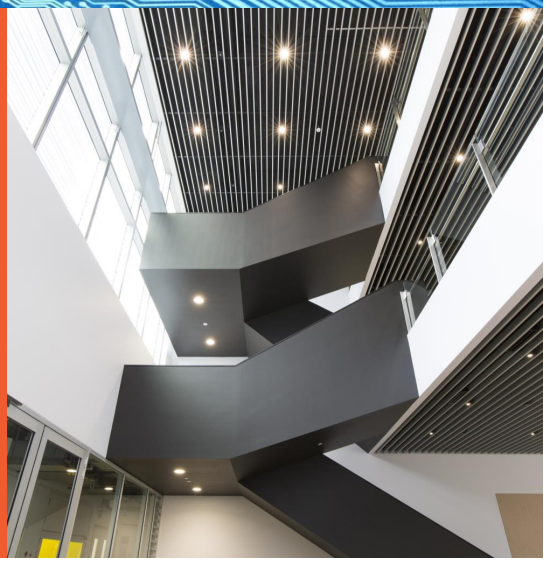
CMP Lecture 15

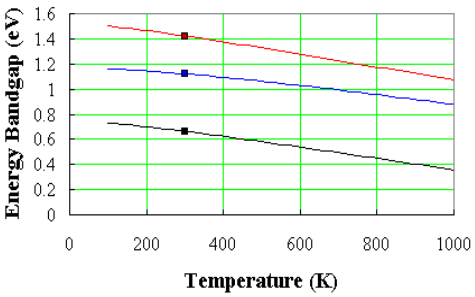
School of Physics
The University of Sydney

THE UNIVERSITY OF SYDNEY



Temperature dependence of the energy bandgap

- The energy bandgap of semiconductors decreases as the temperature is increased.
- Can be understood in that the interatomic spacing increases when the amplitude of the atomic vibrations increases due to the increased thermal energy.
- An increased interatomic spacing decreases the potential seen by the electrons in the material, which in turn reduces the size of the energy gap bandgap.



experimentally determined

	Germanium	Silicon	GaAs
Eg(0) [eV]	0.7437	1.166	1.519

$$E_g(T) = E_g(0) - \frac{\alpha T^2}{T + \beta}$$

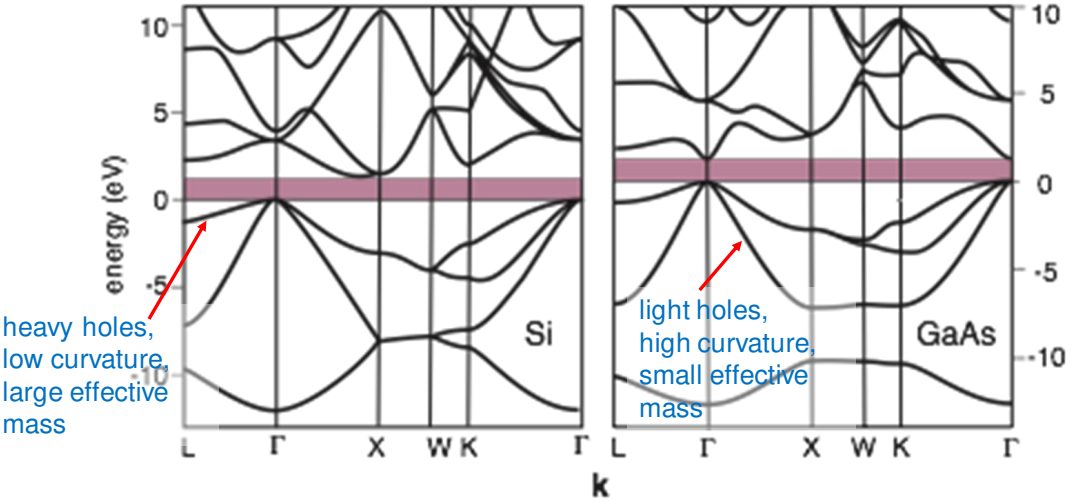
This behaviour could also contribute to the increase in conductivity with temperature.

Ashcroft & Mermin, Ch. 28

Heavy and light holes

Effective mass inversely proportional to the curvature of the band

$$m^* = \hbar^2 \left(\frac{d^2 E(k)}{dk^2} \right)^{-1} > 0$$



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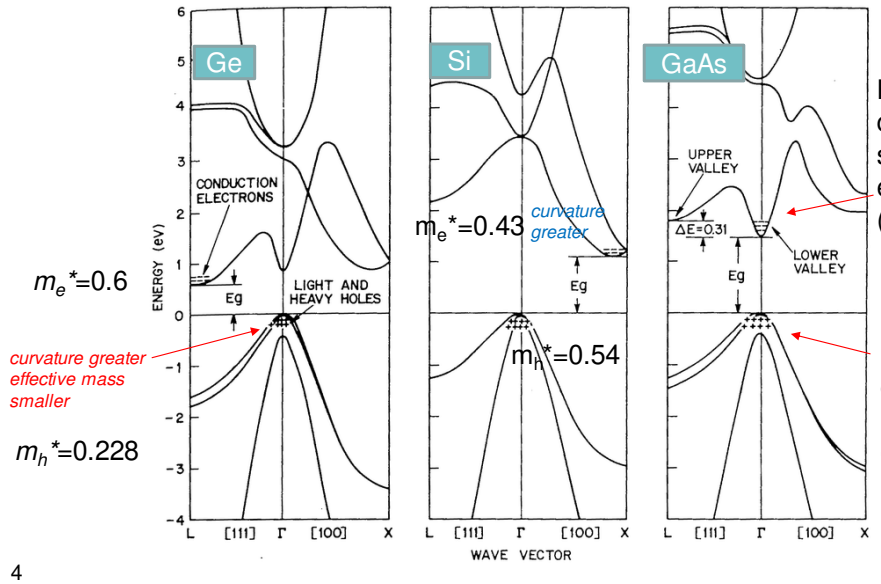


m_e*=0.6

curvature greater effective mass smaller

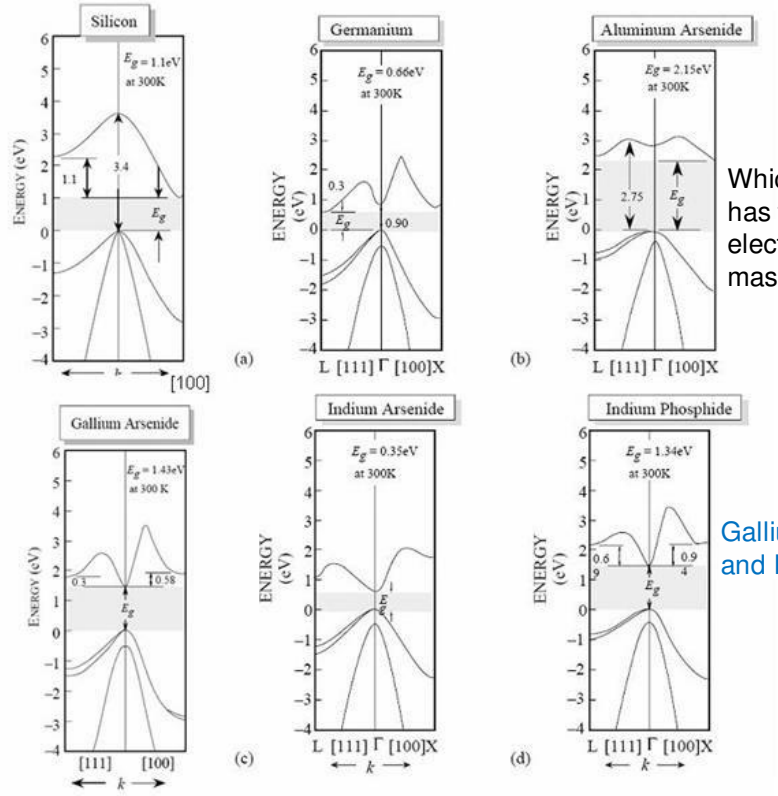
m_h*=0.228

m_e*=0.43 *curvature greater*

m_h*=0.54

High/large curvature, so small effective mass (0.065 m^*_e)

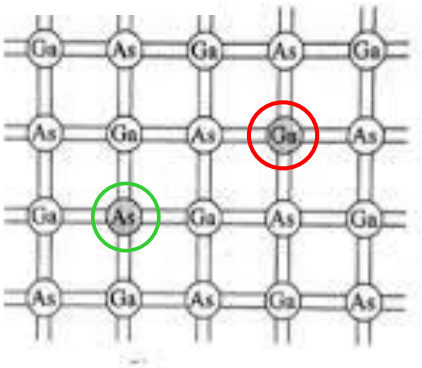
Low/small curvature, so larger effective mass (0.5 m^*_h)



Which semiconductor has the lowest electron effective mass?

Gallium Arsenide and Indium Phosphide

Question: n- and p-type doping Gallium Arsenide

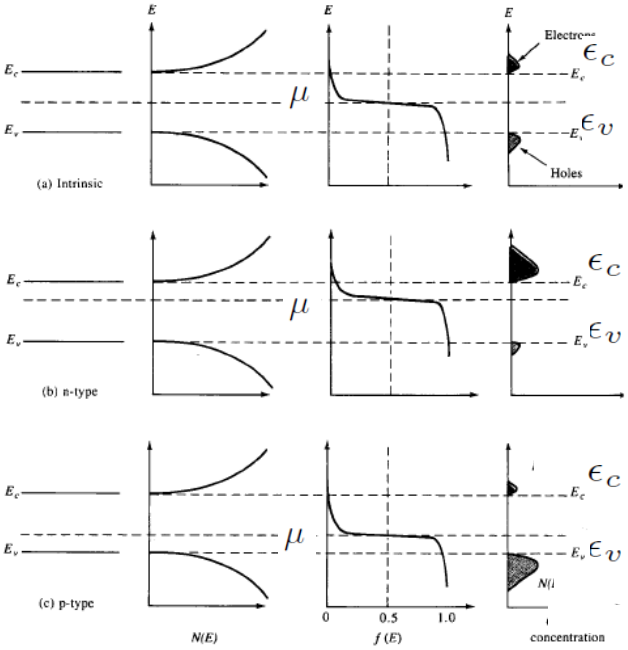


Si: [Ne] $3s^2\ 3p^2$
As: [Ar] $3d^{10}\ 4s^2\ 4p^3$
Ga: [Ar] $3d^{10}\ 4s^2\ 4p^1$

If Si atoms are doped in the system and replace some Ga atoms, will Si-doped GaAs be n-type or p-type?

If the Si atoms replace instead As atoms, will GaAs be n- or p-type?

Band diagram, density of states, Fermi-Dirac distribution, and the carrier concentrations at thermal equilibrium



Intrinsic semiconductor

n-type semiconductor

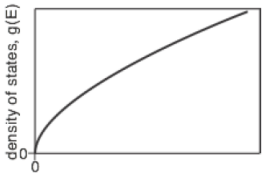
p-type semiconductor

Note: degenerate semiconductor is a one with such a high level of doping that the material starts to act more like a metal than as a semiconductor.

Statistical mechanics of semiconductors

Recall from Lecture 2 – density of states for free electrons per unit volume:

$$g(\epsilon \geqslant 0) = \frac{(2m)^{3/2}}{2\pi^2\hbar^3}\sqrt{\epsilon}$$

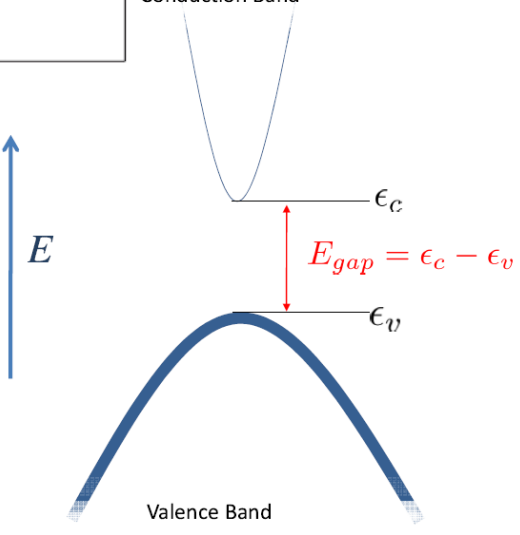


Electrons in conduction band like free electrons but with mass m*, can write:

$$g_c(\epsilon \geqslant \epsilon_c) = \frac{(2m_e^*)^{3/2}}{2\pi^2\hbar^3}\sqrt{\epsilon - \epsilon_c}$$

Similarly the density of states for holes near the top of the valence band are:

$$g_v(\epsilon \leqslant \epsilon_v) = \frac{(2m_h^*)^{3/2}}{2\pi^2\hbar^3}\sqrt{\epsilon_v - \epsilon}$$



The Fermi-Dirac distribution for a semiconductor

Recall: n_F or $f(E) = \dfrac{1}{e^{(E-\mu)/k_B T} + 1}$

It gives the probability that an available energy state *E* will be occupied by an electron at absolute temperature *T*.

- For a metal, the Fermi energy is the highest occupied energy at 0 K.
- For a semiconductor, the definition of the Fermi energy is not so clear. We use the chemical potential μ.
- Some also use the term "Fermi energy" for semiconductors, but then it is temperature-dependent.

Statistical mechanics of semiconductors

For a given chemical potential, the total number of electrons in the conduction band as a function of temperature is:

$$n(T) = \int_{\epsilon_c}^{\infty} d\epsilon\, g_c(\epsilon)\; n_F(\beta(\epsilon - \mu)) = \int_{\epsilon_c}^{\infty} d\epsilon\, \frac{g_c(\epsilon)}{e^{\beta(\epsilon-\mu)} + 1}$$

where $\beta^{-1} = k_B T$

(at room temp. $k_B T$ = 0.025 eV)

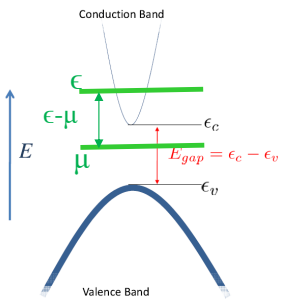
If μ is well below the conduction band, i.e. if

$$\beta(\epsilon - \mu) \gg 1$$

exponential very big; neglect the "1" in denominator

We have $\dfrac{1}{e^{\beta(\epsilon-\mu)} + 1} \approx e^{-\beta(\epsilon-\mu)}$

Boltzman distribution replaces Fermi statistics when T is low enough that that the density of electrons in the band is low



And then,

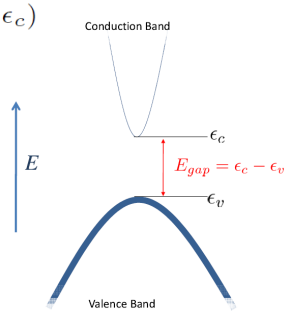
$$= \frac{(2m_e^*)^{3/2}}{2\pi^2\hbar^3} \int_{\epsilon_c}^{\infty} d\epsilon\, (\epsilon - \epsilon_c)^{1/2} e^{-\beta(\epsilon-\mu)} \qquad (1)$$

Statistical mechanics of semiconductors

$$= \frac{(2m_e^*)^{3/2}}{2\pi^2\hbar^3} \int_{\epsilon_c}^{\infty} d\epsilon \, (\epsilon - \epsilon_c)^{1/2} e^{-\beta(\epsilon-\mu)} \quad (1)$$

Want to solve integral: multiply Eq. (1) by $e^{\beta(\mu-\epsilon_c)} \; e^{-\beta(\mu-\epsilon_c)} = 1$

$$= \frac{(2m_e^*)^{3/2}}{2\pi^2\hbar^3} e^{\beta(\mu-\epsilon_c)} \int_{\epsilon_c}^{\infty} d\epsilon \, (\epsilon - \epsilon_c)^{1/2} e^{-\beta(\epsilon-\epsilon_c)}$$



Standard Equation for density of electrons

$$n(T) = \frac{1}{4}\left(\frac{2m_e^* k_B T}{\pi\hbar^2}\right)^{3/2} e^{-\beta(\epsilon_c-\mu)}$$

Electrons are activated from the chemical potential up into the conduction band

Working

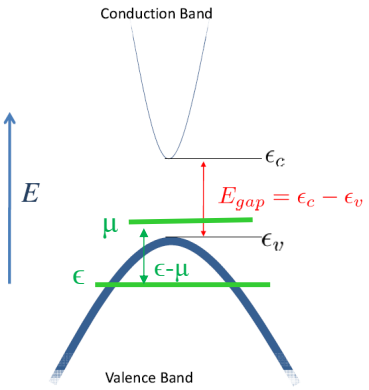
Statistical mechanics of semiconductors

Similarly can get the number of holes *p* in the valence band as:

$$p(T) = \int_{-\infty}^{\epsilon_v} d\epsilon\, g_v(\epsilon)\left[1 - \frac{1}{e^{\beta(\epsilon-\mu)}+1}\right]$$

$$= \int_{-\infty}^{\epsilon_v} d\epsilon\, \frac{g_v(\epsilon)e^{\beta(\epsilon-\mu)}}{e^{\beta(\epsilon-\mu)}+1}$$

If the Fermi function n_F gives the prob. a state is occupied by an electron, then $1 - n_F$ gives the prob. that the state is occupied by a hole.



When μ substantially above the top of the valence band we have:

$$e^{\beta(\epsilon-\mu)} \ll 1$$

and

$$p(T) = \int_{-\infty}^{\epsilon_v} d\epsilon\, g_v(\epsilon) e^{\beta(\epsilon-\mu)}$$

Standard Equation for density of holes

$$p(T) = \frac{1}{4}\left(\frac{2m_h^* k_B T}{\pi\hbar^2}\right)^{3/2} e^{-\beta(\mu-\epsilon_v)}$$

Holes are activated from the chemical potential down into the valence band

Law of Mass Action

Forming product of density of electrons in conduction band and holes in the valence band we obtain important relation:

$$n(T)p(T) = \frac{1}{2}\left(\frac{k_B T}{\pi\hbar^2}\right)^3 (m_e^*\, m_h^*)^{3/2}\, e^{-\beta(\epsilon_c-\epsilon_v)}$$

$$= \frac{1}{2}\left(\frac{k_B T}{\pi\hbar^2}\right)^3 (m_e^*\, m_h^*)^{3/2}\, e^{-\beta E_{gap}}$$

Depends on band gap $E_{gap} = \epsilon_c - \epsilon_v$

Intrinsic semiconductors

Number of electrons excited into conduction band must equal number of holes left behind in valence band so $p = n$.

Dividing the density of electrons in conduction band *n(T)*, and holes in the valence band *p(T)* we obtain:

$$1 = \left(\frac{m_e^*}{m_h^*}\right)^{3/2} e^{-\beta(\epsilon_v+\epsilon_c-2\mu)}$$

Intrinsic semiconductors

Taking the log of both sides of the below

$$1 = \left(\frac{m_e^*}{m_h^*}\right)^{3/2} e^{-\beta(\epsilon_v+\epsilon_c-2\mu)}$$

and solving for μ gives:

$$\mu = \frac{1}{2}(\epsilon_c + \epsilon_v) + \frac{3}{4}(k_B T)\log(m_h^*/m_e^*)$$

This is an expression for the chemical potential – at *T=0* gives it exactly in the **middle of the band-gap**.

Using the law of Mass Action above with *n=p* we obtain:

$$n_{intrinsic} = p_{intrinsic} = \sqrt{np} = \frac{1}{\sqrt{2}}\left(\frac{k_B T}{\pi\hbar^2}\right)^{3/2} (m_e^*\, m_h^*)^{3/4}\, e^{-\beta E_{gap}/2}$$

Extrinsic/doped semiconductors

Law of Mass Action also holds for doping when we have concentrations *n* and *p*.

(see Oxford Basics p. 193 for details)

Consider intrinsic case:

$$I = n_{intrinsic} = p_{intrinsic}$$

From the law of mass action we have product of electron and hole concentrations, equals square of intrinsic concentration.

$$np = I^2 = \frac{1}{2}\left(\frac{k_B T}{\pi\hbar^2}\right)^3 (m_e^*\, m_h^*)^{3/2}\, e^{-\beta E_{gap}}$$

Example

Using prefactor $N_{\text{eff}}^{C} = 10^{25}\text{m}^{-3}$

$$n_{intrinsic} = p_{intrinsic} = \sqrt{np} = \frac{1}{\sqrt{2}} \left(\frac{k_B T}{\pi \hbar^2} \right)^{3/2} (m_e^* \, m_h^*)^{3/4} \, e^{-\beta E_{gap}/2}$$

	gap size (eV)	n in m^{-3} at 150 K	n in m^{-3} at 300 K
InSb	0.18	2×10^{22}	6×10^{23}
Si	1.11	4×10^{6}	2×10^{16}
diamond	5.5	6×10^{-68}	1×10^{-21}

Remember: metal is about 10^{28} per m^3

InSb: high and fairly constant. Si: strongly T-dep; from almost nothing to something relevant. Diamond: dramatic but irrelevant

Example question

Consider a Si sample at $T = 300$ K, doped with Boron to a concentration 2×10^{16} cm^{-3}.

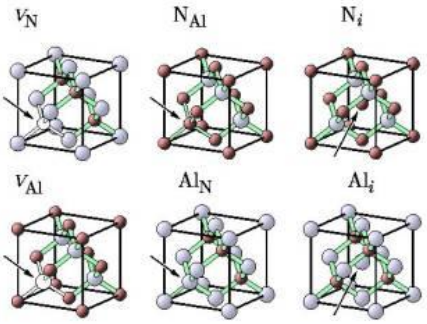
Given the intrinsic concentration $n_i = p_i$ is 1×10^{10} cm^{-3}, what are the electron and hole concentrations (n and p) in this sample? Is it n-type or p-type?

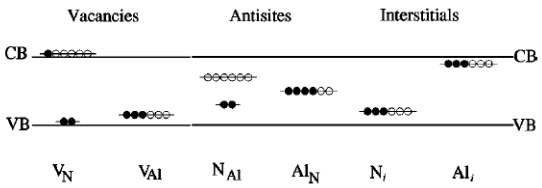
Example question

Suppose the sample is doped additionally with phosphorus to a concentration 6×10^{16} cm^{-3}.
Is the material now n-type or p-type? What are the *n* and *p* concentrations now?

Native defects in AlN: example

Electronic structure calculations





Give rise to various states in the band gap

Consider typical native (intrinsic) defects

But how likely are these defects to form?

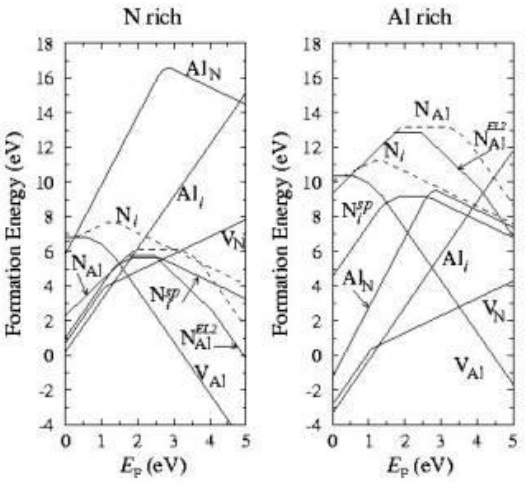
Native defects in AlN

Can calculate formation energies

$$E^f(q) = E^{\text{tot}}_{\text{defect}}(q) - E^{\text{tot}}(\text{bulk}) - n_{\text{Al}}\mu_{\text{Al}} - n_{\text{N}}\mu_{\text{N}} + qE_F$$

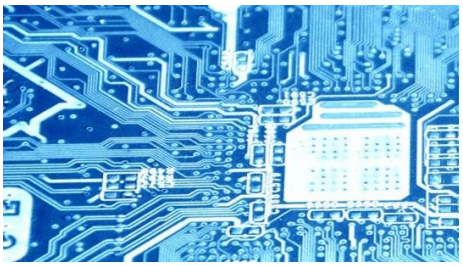
as function of position of chemical potential (of "Fermi level").

V_N has the lowest formation energy in *p*-type material (near $E_F = 0$, i.e. near the valence band maximum) and the aluminium vacancy, V_{Al}, has the lowest formation energy in n-type material (near $E_F = 5$, i.e. closer to the conduction band minimum).



PHYSICAL REVIEW B, VOLUME 65, 155212

Semiconductor devices



The development of semiconductor electronic devices constitutes perhaps the greatest technological advance of the modern era.

This entire industry owes its very existence to our detailed understanding of quantum condensed matter physics.

Invention of the transistor was due to the Bell Labs (famous labs located near New York) team of J. Bardeen, W. Brattain, and W. Shockley in 1947. Received the Nobel Prize for this. Perhaps the most important invention of the 20th century.
Bardeen left Bell Labs to the University of Illinois, Champagne-Urbana, where he started work on the theory of superconductivity, for which he won a **second** Nobel Prize (BSC theory).

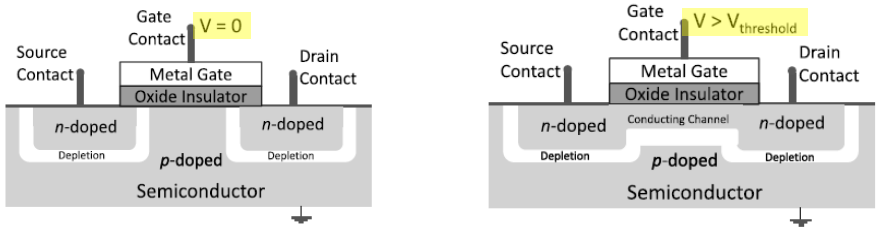
Every iPad, iPhone contains billions of transistors

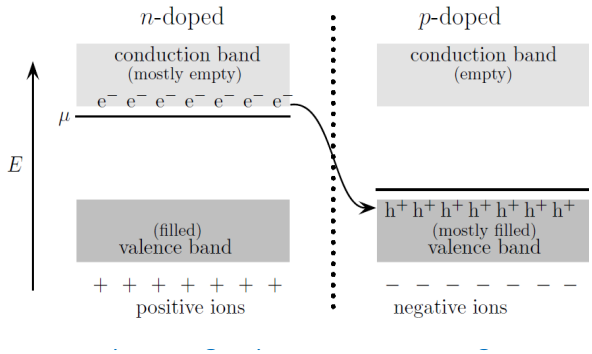
n-MOSFET transistor

Oxford Basics, Ch. 18

acts as a switch or amplifier

Usually a combination of n- and p-type MOSFETS are on the same chip – called "complementary MOS logic" - CMOS





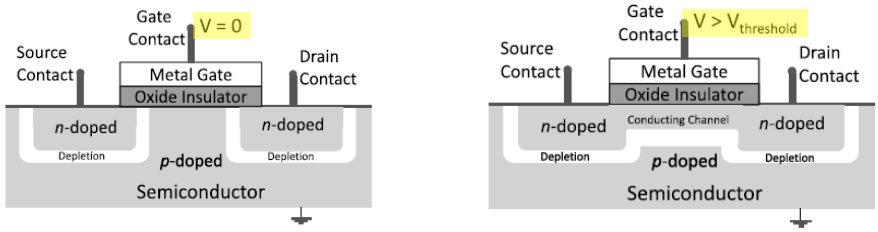
Depletion layer is region formed between n- and p-type material.
In n-type μ is near the top of the band-gap. In p-type μ is near the bottom of the band-gap.
When the two materials are brought into contact, electrons in the conduction band fall into the valence band, filling the empty hole states and pair-annihilating creating a region with no carriers.

n-MOSFET transistor

Oxford Basics, Ch. 18

acts as a switch or amplifier

Usually a combination of n- and p-type MOSFETS are on the same chip – called "complementary MOS logic" - CMOS



When a positive voltage is applied to the metal gate, it attracts negative charge to the region just under the oxide insulator. This attraction of charge is known as a "field effect", since it is the result of an electric field caused by the gate.

If the gate voltage larger than some particular threshold voltage the region under the gate becomes effectively n-like. Then there is a continuous channel of n-semiconductor that stretches from the source to the drain and the conductance between source and drain becomes very large.

Thus, a small voltage on the gate can control a large current between the source and drain, hence providing amplification of small signals.

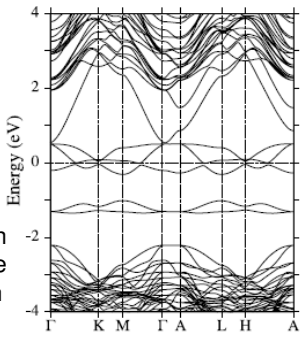
Semiconductors for spintronics

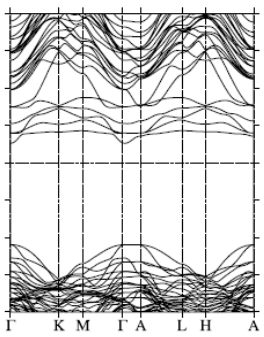
Half-Metallicity and Efficient Spin Injection in AlN/GaN:Cr (0001) Heterostructure

Phys. Rev. Lett. **94**, 146602

Doping can lead to magnetic effects in non-magnetic semiconductors

Spin-down





Spin-up

Spintronics is also known as spin electronics, is the study of the intrinsic spin of the electron and its associated magnetic moment, in addition to its fundamental electronic charge.

Spintronics is the alternative future technology, which is based on using the fundamental spin of electron in additions to its charge to carry and store information.

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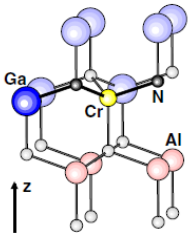

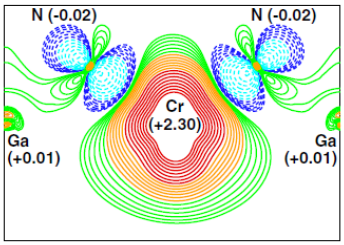

End