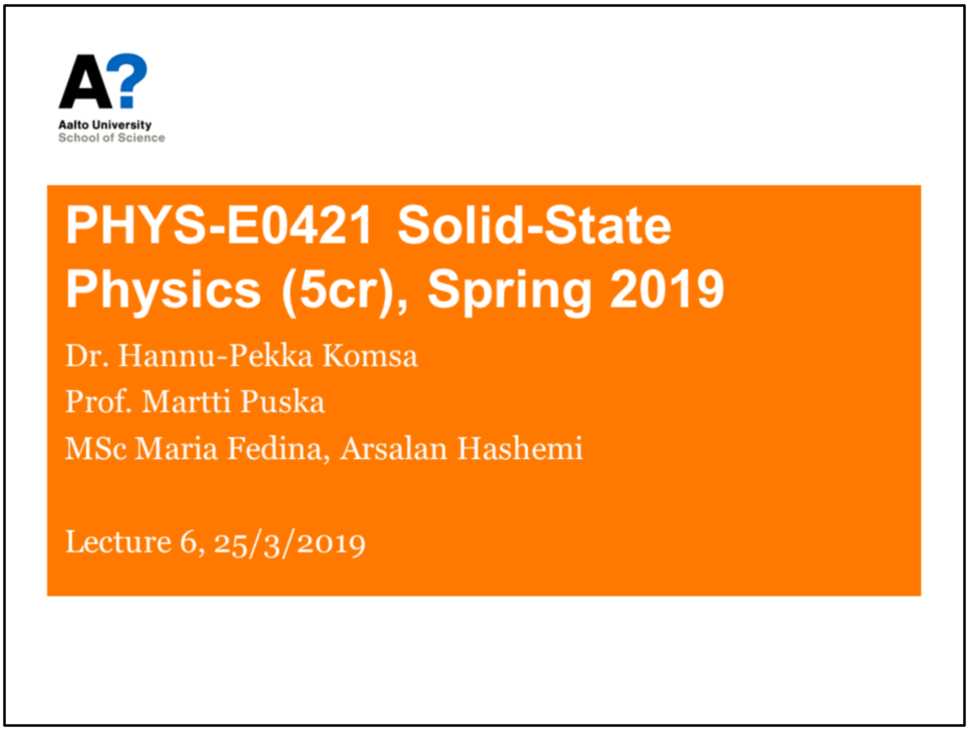

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PHYS-E0421 Solid-State Physics (5cr), Spring 2019

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Lecture 6, 25/3/2019

Today's topics

Some main ideas and principles of semiconductor technology,

- Semiconductor junctions
  - Semiconductor-metal junction / Schottky barrier and diode
  - Semiconductor heterojunctions + superlattices and quantum wells
  - Semiconductor homojunctions such as the *p-n* junction
- Examples of devices utilizing the above structures and ideas

A summary of related learning objectives:

- Understanding how band diagrams of the junctions look like and why, where the charge carriers can be found and how they move, behavior in non-equilibrium situations (external bias)
- Understanding phenomena characteristic for small-scale devices in reduced dimensions (quantum confinement etc.)
- Ability to describe the principle of operation of a simple device (*p-n* junction, Schottky diode, metal-oxide semiconductor device, solar cell or light-emitting diode)

(See also the questions on the slides!)

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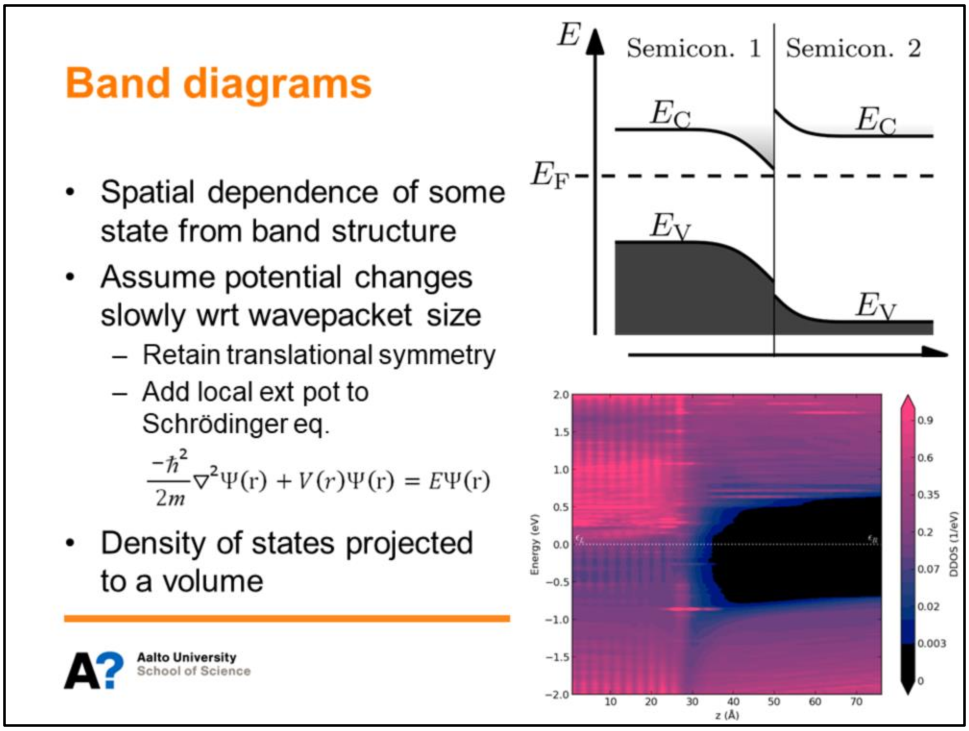

Band diagrams

- Spatial dependence of some state from band structure
- Assume potential changes slowly wrt wavepacket size
  - Retain translational symmetry
  - Add local ext pot to Schrödinger eq.

$$\frac{-\hbar^2}{2m}\nabla^2\Psi(\mathrm{r}) + V(r)\Psi(\mathrm{r}) = E\Psi(\mathrm{r})$$

- Density of states projected to a volume

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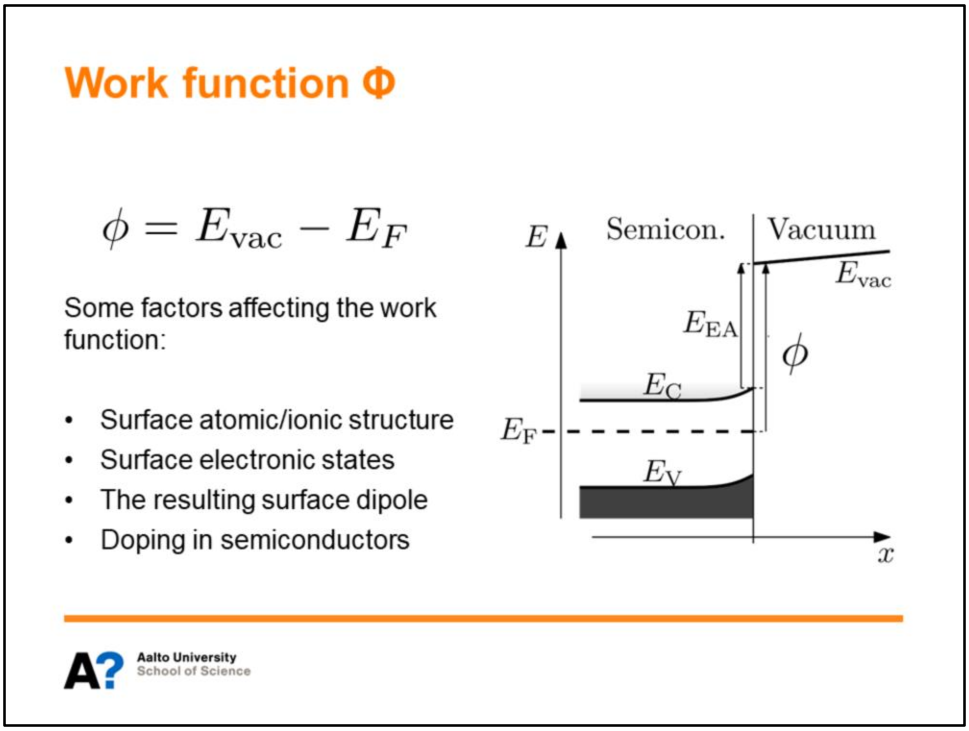
- Valence and conduction band edges as a function of spatial position, taken from the maximum/minimum in k-space. (+defect states)
- Projected DOS: around position r, weight the DOS by |psi(r)|^2, where psi are the states that contribute to the DOS at the given energy.



Work function Φ

$$\phi = E_{\text{vac}} - E_F$$

Some factors affecting the work function:

- Surface atomic/ionic structure
- Surface electronic states
- The resulting surface dipole
- Doping in semiconductors

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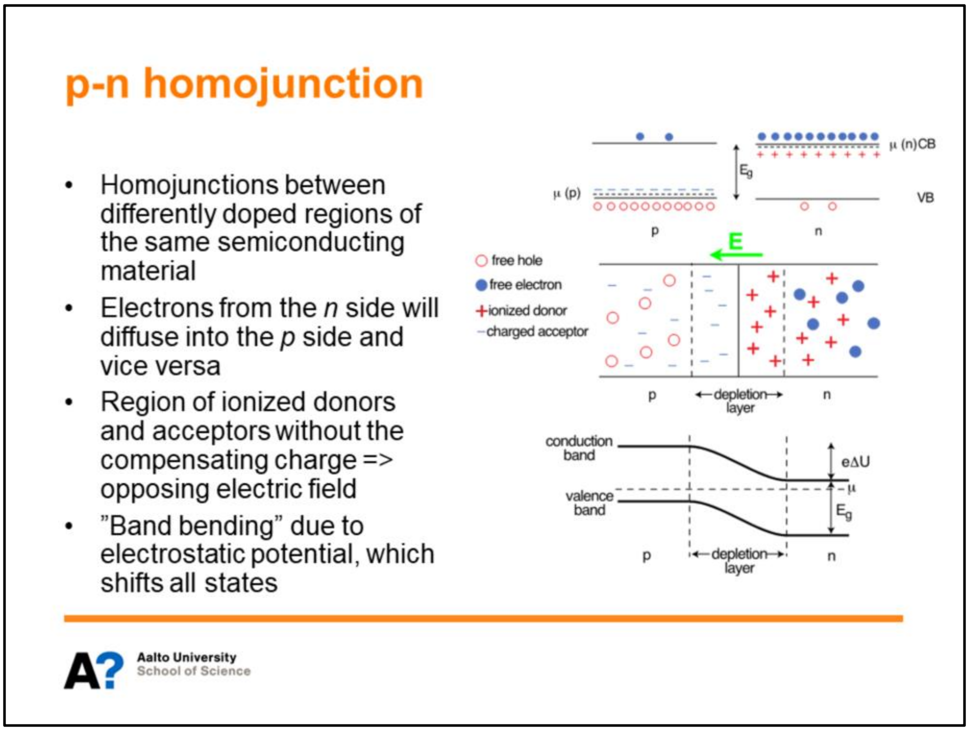
- Aligns the band structures before forming the junctions
- Ionization potential: Evac-Ev



p-n homojunction

- Homojunctions between differently doped regions of the same semiconducting material
- Electrons from the *n* side will diffuse into the *p* side and vice versa
- Region of ionized donors and acceptors without the compensating charge => opposing electric field
- ”Band bending” due to electrostatic potential, which shifts all states

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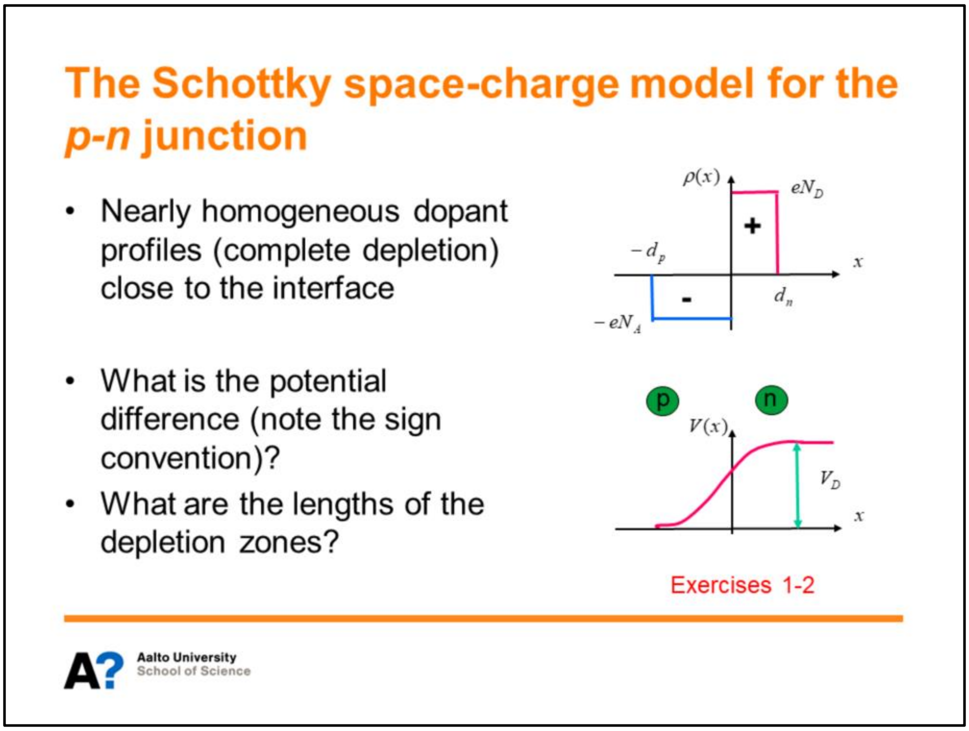
- Either: 1) electrons and holes at the two sides of the interface recombine, or 2) electrons from n-side fill the acceptors on p-side, and leave behind ionized donors
- Generation of electric field opposing the charge transfer => Fermi-levels are aligned (or rather electrochemical potential)
- We could solve Schrödinger equation for the whole system and determine global chemical potential, or we can solve SE locally under external electrostatic potential and search for solution where electrochemical potential is aligned throughout the system.
- Small number of free carriers => Fermi-level far away from band edges. Or: within the depletion layer, Fermi-level in the saturation regime, all dopants are ionized.



The Schottky space-charge model for the *p-n* junction

- Nearly homogeneous dopant profiles (complete depletion) close to the interface
- What is the potential difference (note the sign convention)?
- What are the lengths of the depletion zones?

Exercises 1-2

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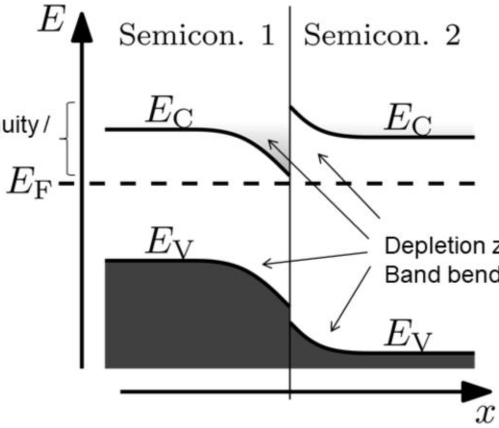
- Potential from solution of 1D Poisson equation
- The extent of band bending depends on the dopant concentrations, longer if small concentration

Semiconductor-semiconductor heterojunction



Band discontinuity / Band offset

Depletion zone / Band bending

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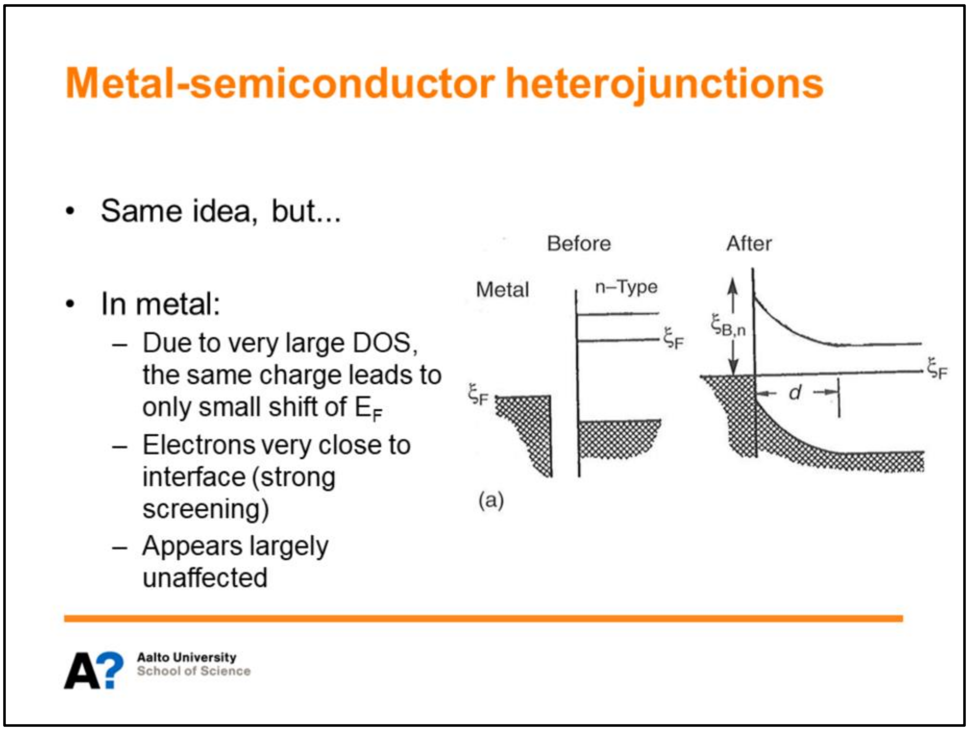
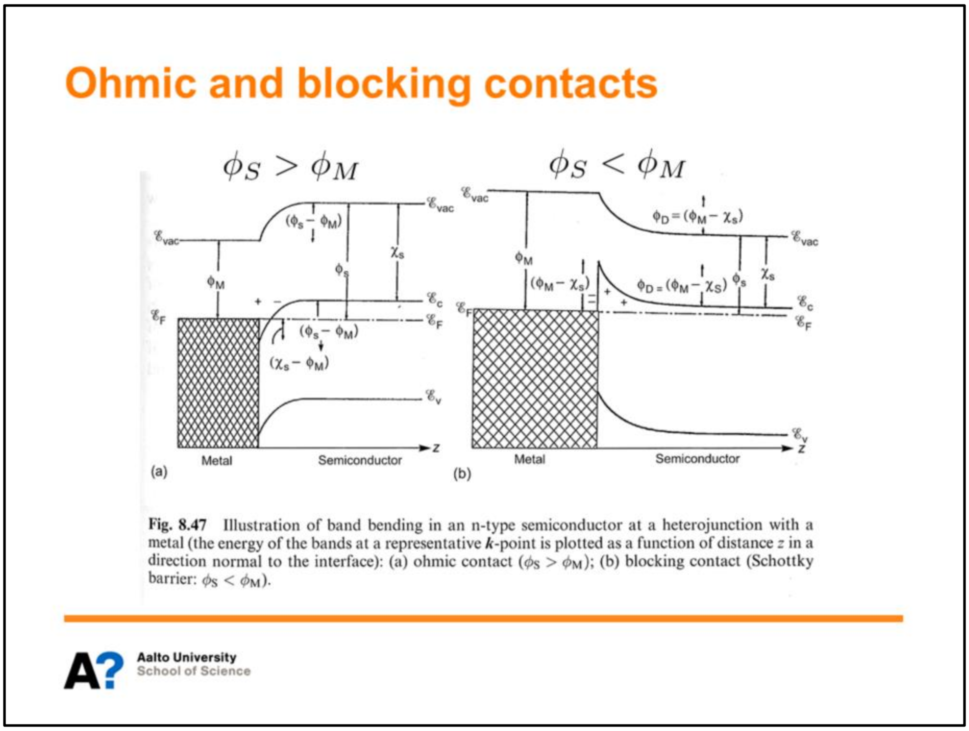


Metal-semiconductor heterojunctions

- Same idea, but...
- In metal:
  - Due to very large DOS, the same charge leads to only small shift of E_F
  - Electrons very close to interface (strong screening)
  - Appears largely unaffected

- Transfer of electrons from higher Fermi-level to lower => electric field, band bending, Fermi-level drops
- In the metal side, similar effects, but confined to a region very close to the interface
- For our purpose, there are no special bands in metal, like VB/CB in semicond, but shift can be seen e.g. in core states.
- Remember the local DOS figure in the beginning.



Ohmic and blocking contacts

Fig. 8.47 Illustration of band bending in an n-type semiconductor at a heterojunction with a metal (the energy of the bands at a representative ***k***-point is plotted as a function of distance *z* in a direction normal to the interface): (a) ohmic contact ($\phi_S > \phi_M$); (b) blocking contact (Schottky barrier: $\phi_S < \phi_M$).

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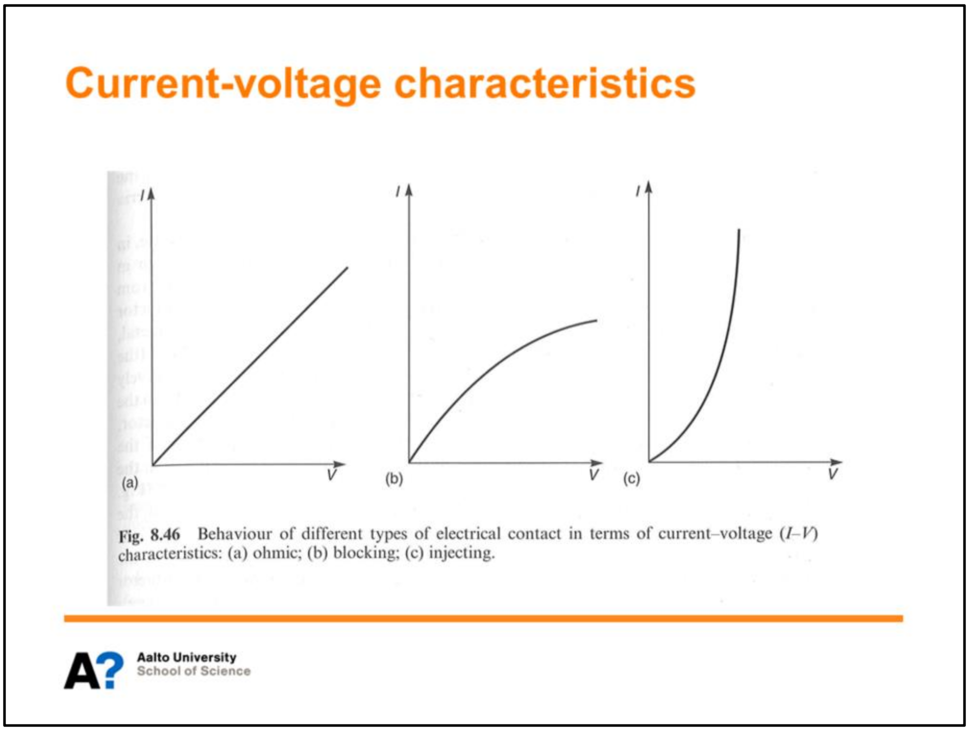
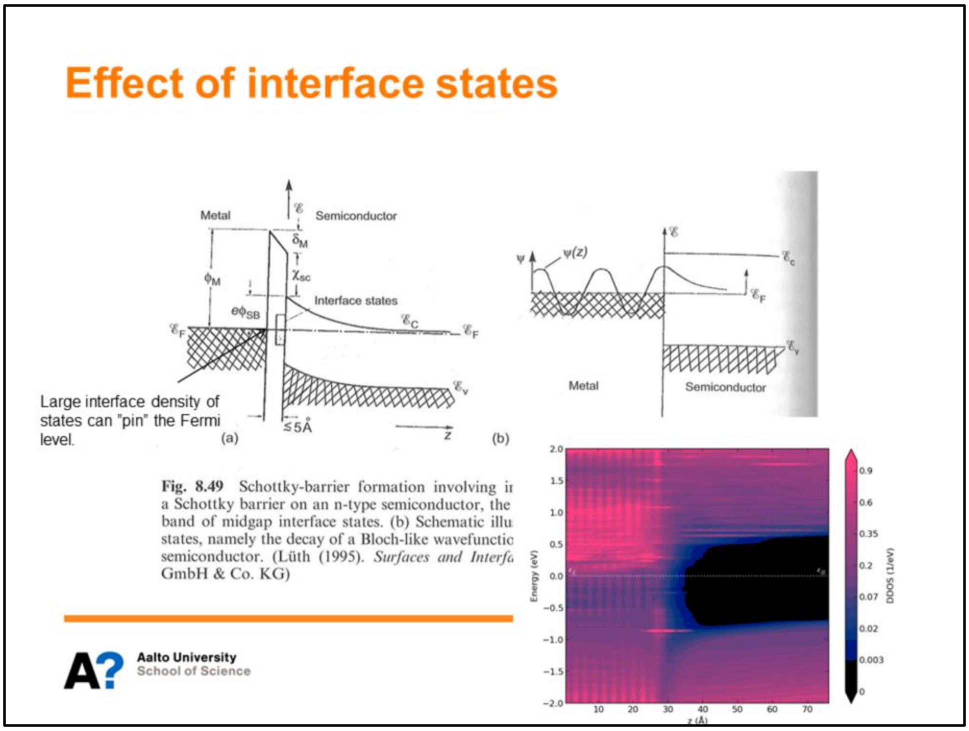
- Type of contact depends on the doping and relative position of Fermi-level
- No barriers in Ohmic contact, easy charge flow. Semiconductor is degenerate at the interface.
- Barrier in Schottky contact, thermal excitations or tunneling needed
- Often, sufficiently Ohmic contact is obtained by doping the interface very heavily which makes the barrier very thin and carriers can tunnel through
- Ohmic for electrons is Schottky for holes, and vice versa, although mostly only the type for majority carrier matters



Current-voltage characteristics

Fig. 8.46 Behaviour of different types of electrical contact in terms of current–voltage (I–V) characteristics: (a) ohmic; (b) blocking; (c) injecting.

- Strangely explained in the book, IMO.
- (b) and (c) both happen in ”blocking” metal-semiconductor interface depending on the bias.



Effect of interface states

Large interface density of states can "pin" the Fermi level.

Fig. 8.49 Schottky-barrier formation involving i
a Schottky barrier on an n-type semiconductor, the
band of midgap interface states. (b) Schematic illu
states, namely the decay of a Bloch-like wavefunctio
semiconductor. (Lüth (1995). *Surfaces and Interfa*
GmbH & Co. KG)

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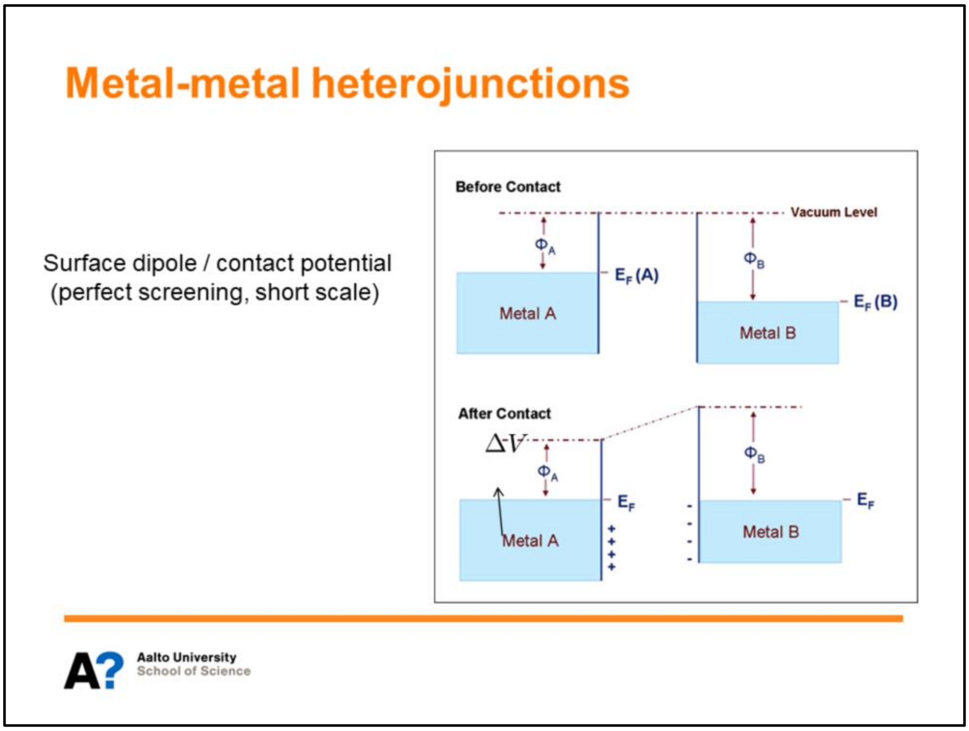
- Interface states from the breaking of lattice, kind of defect states, depends on details of the interface
- MIGS, figure of DOS smoothing, compare tunneling through simple barrier in quantum mechanics
- Fermi-level pinning affects Schottky barrier and band bending. E.g., barrier becomes independent of the metal work function.



Metal-metal heterojunctions

Surface dipole / contact potential
(perfect screening, short scale)

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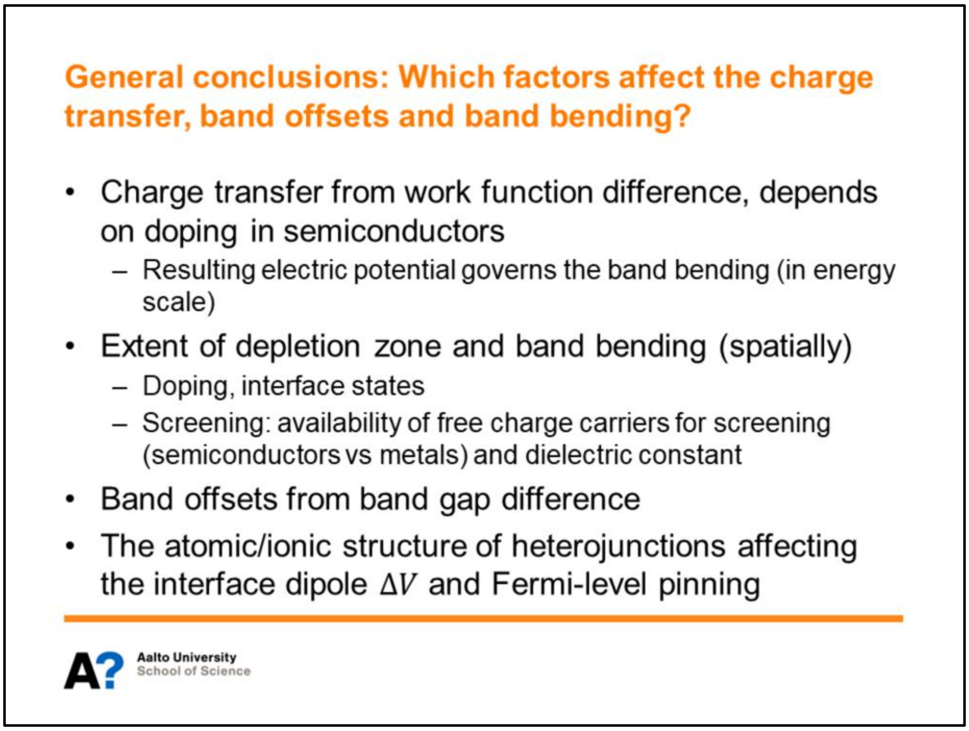
- Any potential originating from the charge transfer is quickly screened out further away from the junction
- Due to large DOS, the electrons can stay close to the junction without having to go much higher in (kinetic) energy



General conclusions: Which factors affect the charge transfer, band offsets and band bending?

- Charge transfer from work function difference, depends on doping in semiconductors
  - Resulting electric potential governs the band bending (in energy scale)
- Extent of depletion zone and band bending (spatially)
  - Doping, interface states
  - Screening: availability of free charge carriers for screening (semiconductors vs metals) and dielectric constant
- Band offsets from band gap difference
- The atomic/ionic structure of heterojunctions affecting the interface dipole ΔV and Fermi-level pinning

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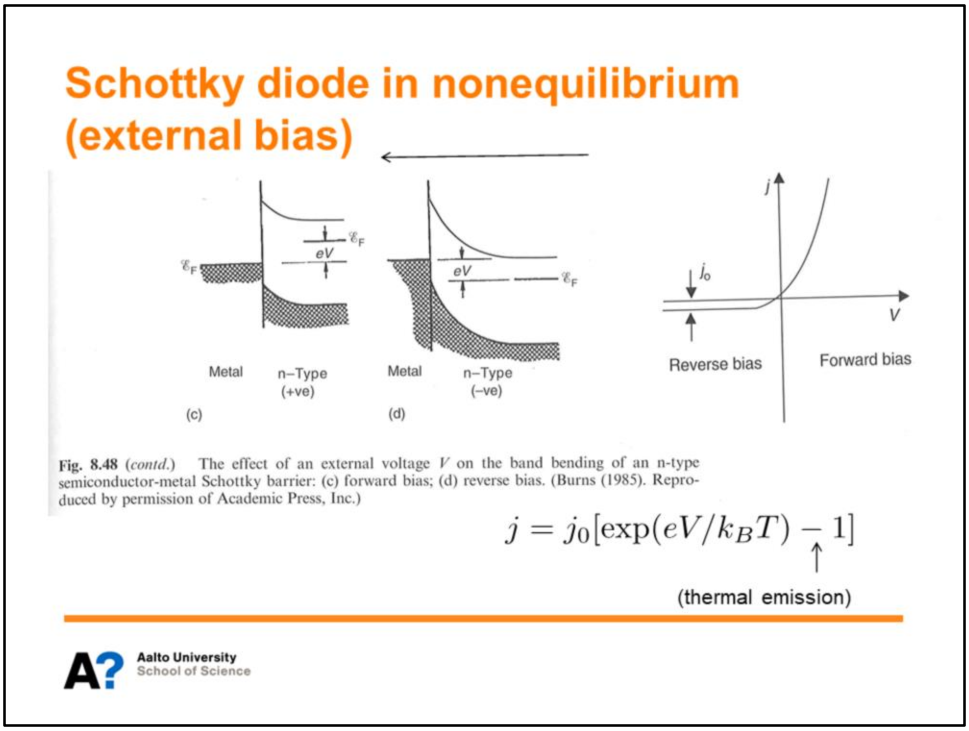
- First question was in homework.



Schottky diode in nonequilibrium (external bias)

Fig. 8.48 (*contd.*) The effect of an external voltage V on the band bending of an n-type semiconductor-metal Schottky barrier: (c) forward bias; (d) reverse bias. (Burns (1985). Reproduced by permission of Academic Press, Inc.)

$$j = j_0[\exp(eV/k_BT) - 1]$$

(thermal emission)

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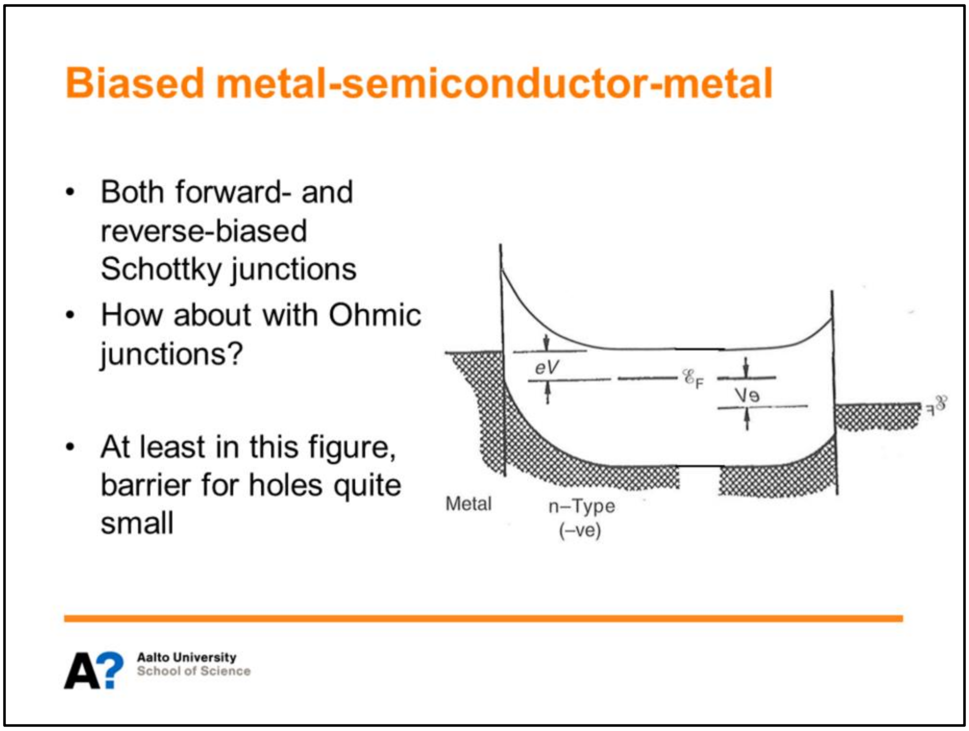
- From j=sigma*E, to have same current in metal and SC, E (=potential gradient) needs to be much larger in SC, since sigma is much smaller.
- Here, the biggest potential drop happens at the junction, where the number of carriers and thus conductivity is smallest. Also screening is small.
- Or, forwards bias decreases the work function difference and thus the required potential change. The opposite for reverse bias.



Biased metal-semiconductor-metal

- Both forward- and reverse-biased Schottky junctions
- How about with Ohmic junctions?

- At least in this figure, barrier for holes quite small

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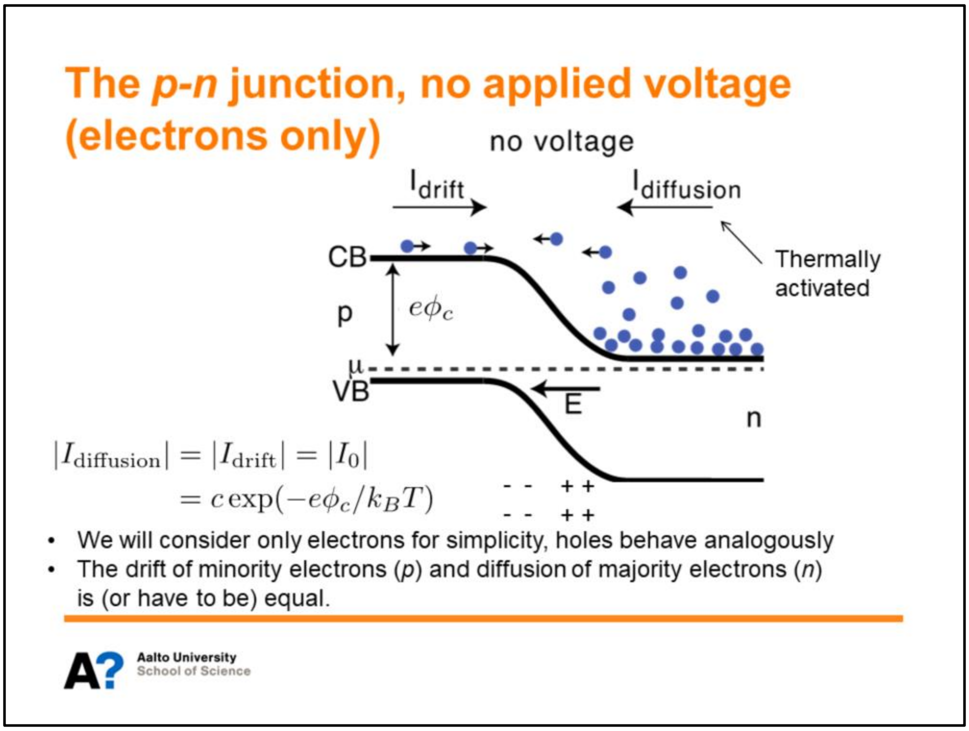
- Large number of holes in n-type semiconductor can lead to strong recombination.



The *p-n* junction, no applied voltage (electrons only)

$$|I_{\text{diffusion}}| = |I_{\text{drift}}| = |I_0|$$
$$= c\exp(-e\phi_c/k_B T)$$

- We will consider only electrons for simplicity, holes behave analogously
- The drift of minority electrons (*p*) and diffusion of majority electrons (*n*) is (or have to be) equal.

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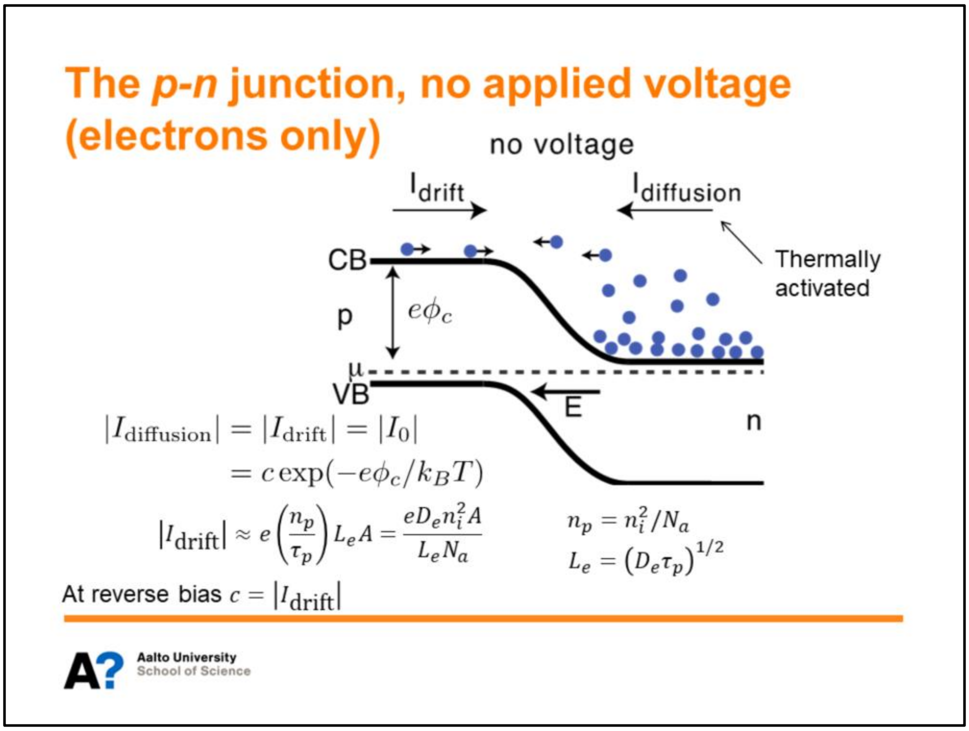
- Drift current due to contact potential and diffusion due to thermal activation over the barrier (or diffusion due concentration gradient)



The *p-n* junction, no applied voltage (electrons only)

$$|I_{\text{diffusion}}| = |I_{\text{drift}}| = |I_0| = c\exp(-e\phi_c/k_BT)$$

$$|I_{\text{drift}}| \approx e\left(\frac{n_p}{\tau_p}\right)L_eA = \frac{eD_en_i^2A}{L_eN_a}$$

$n_p = n_i^2/N_a$

$L_e = \left(D_e\tau_p\right)^{1/2}$

At reverse bias $c = |I_{\text{drift}}|$

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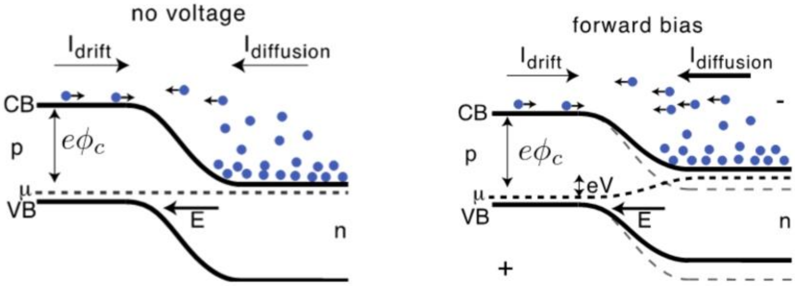
- In drift current: diffusion of electrons to the contact region and replenishing by thermal generation (or prior to recombination).
- The n_p/tau_p term is recombination (=generation) rate

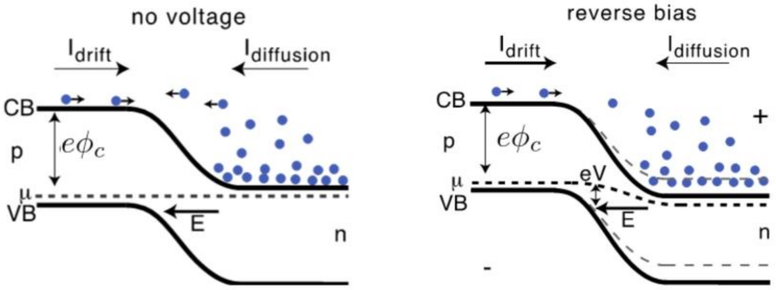
The *p-n* junction with a forward bias (electrons only)



- Voltage drop only over depletion zone (screening elsewhere).
- Increased diffusion current, drift current unaffected.

$$|I_{\text{diffusion}}| = c\exp(-e(\phi_c - V)/k_BT)$$

The *p-n* junction with a reverse bias (electrons only)



- Voltage drop only over depletion zone (screening elsewhere)
- Decreased diffusion current, drift current unaffected.

$$|I_{\text{diffusion}}| = c\exp(-e(\phi_c + V)/k_B T)$$

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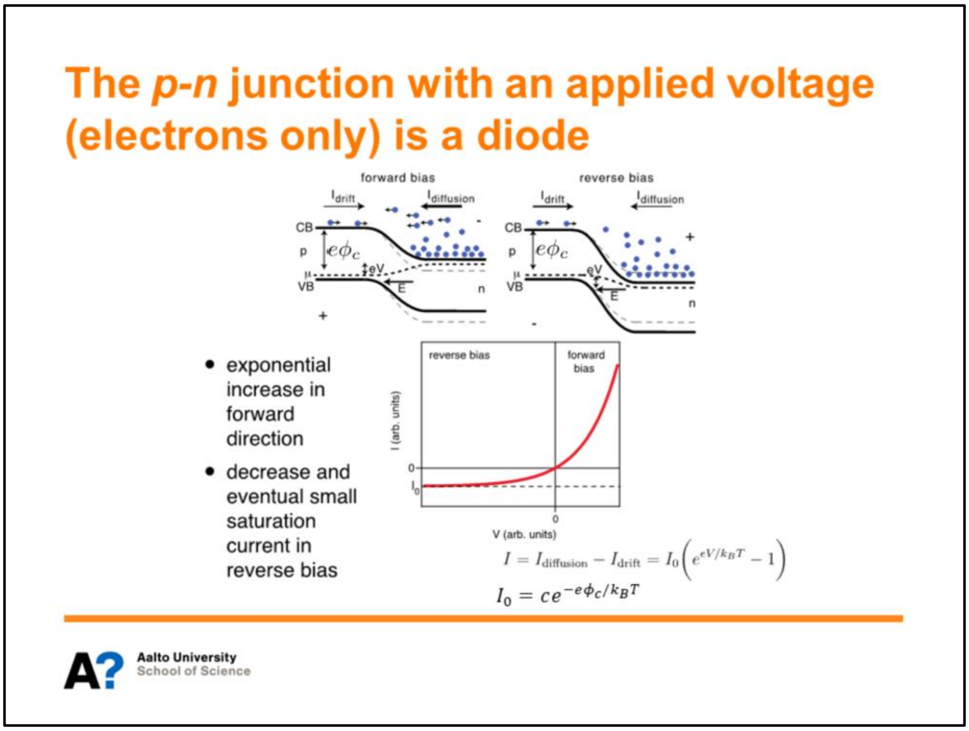

The *p-n* junction with an applied voltage (electrons only) is a diode

- exponential increase in forward direction
- decrease and eventual small saturation current in reverse bias

$$I = I_{\text{diffusion}} - I_{\text{drift}} = I_0\left(e^{eV/k_BT} - 1\right)$$

$$I_0 = ce^{-e\phi_c/k_BT}$$

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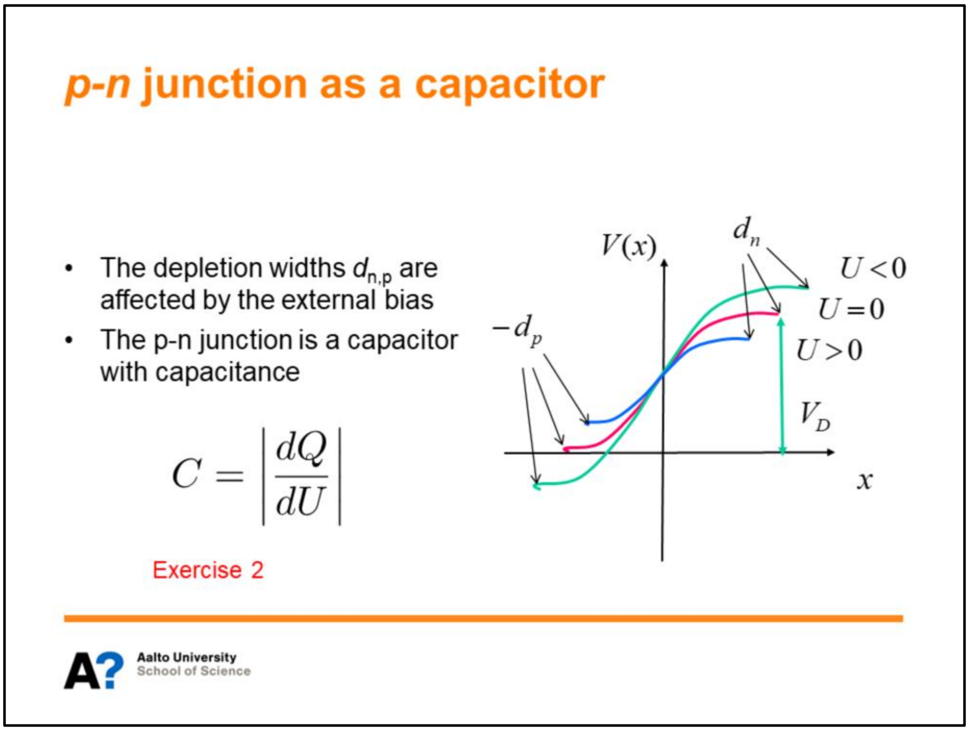
- But not an ideal one diode.
- When accounting also for holes, just sum the electron and hole currents.
- The relative importance of electron and hole currents can be controlled by the doping of the n- and p-sides, see the dependence on N_d/N_a. E.g. N_a < N_d, electrons dominate both drift and diffusion.



p-n junction as a capacitor

- The depletion widths $d_{n,p}$ are affected by the external bias
- The p-n junction is a capacitor with capacitance

$$C = \left|\frac{dQ}{dU}\right|$$

Exercise 2

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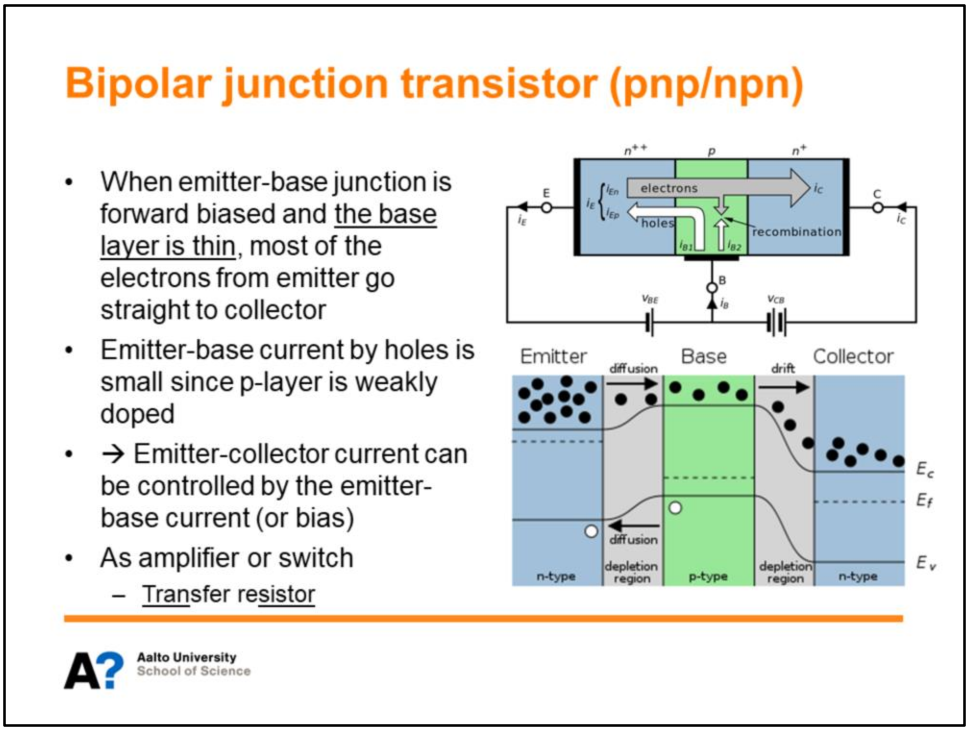
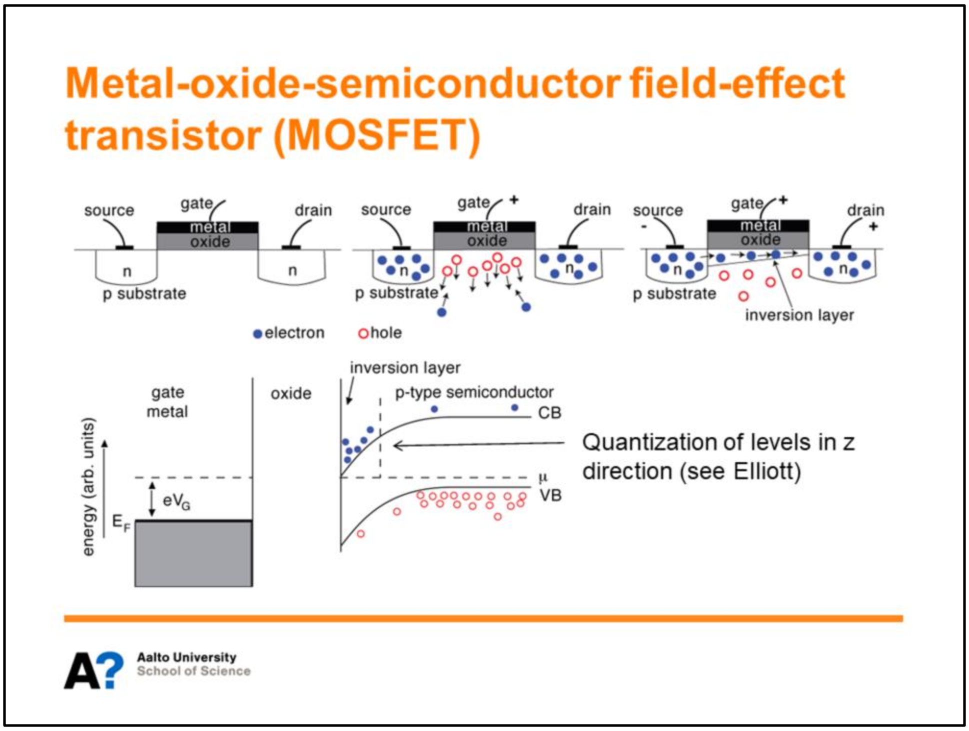
- Contact potential comes from the (integrated) charges in the depletion ragion. Width of the depletion region increases with reverse bias and vice versa.
- One can think that there is built-in capacitance even in the unbiased case. In practice only the differential matters.



Bipolar junction transistor (pnp/npn)

- When emitter-base junction is forward biased and the base layer is thin, most of the electrons from emitter go straight to collector
- Emitter-base current by holes is small since p-layer is weakly doped
- → Emitter-collector current can be controlled by the emitter-base current (or bias)
- As amplifier or switch
  - Transfer resistor

- Perhaps easier to understand so that we control the height of the barrier. This leads also to current, but the current is small due to weak p-doping.
- Weak p-doping => weak recombination
- Bending in p-region extends relatively far due to weak doping vs n-regions.
- Here for npn, pnp analogously



Metal-oxide-semiconductor field-effect transistor (MOSFET)

Quantization of levels in z direction (see Elliott)

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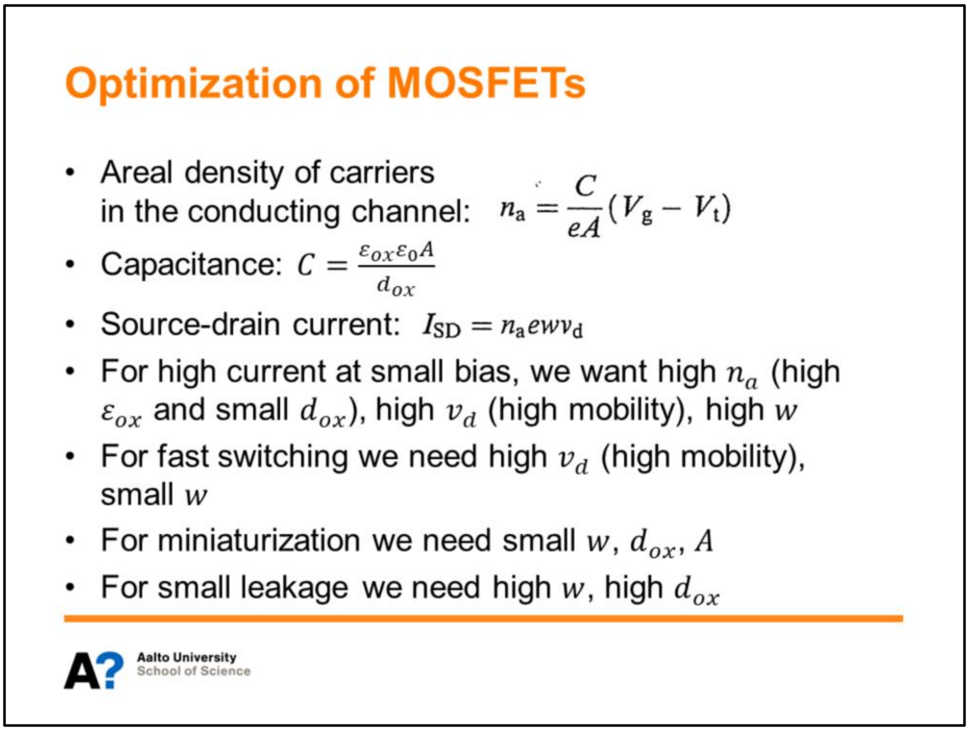
- Band diagram looks a lot like npn-BJT along the interface from source to drain
- Requires good quality of the interface to avoid scattering from defects or roughness
- Controlling gate voltage, source-drain current can be switched on/off



Optimization of MOSFETs

- Areal density of carriers in the conducting channel: $n_\mathrm{a} = \frac{C}{eA}(V_\mathrm{g} - V_\mathrm{t})$
- Capacitance: $C = \frac{\varepsilon_{ox}\varepsilon_0 A}{d_{ox}}$
- Source-drain current: $I_\mathrm{SD} = n_\mathrm{a} e w v_\mathrm{d}$
- For high current at small bias, we want high n_a (high ε_{ox} and small d_{ox}), high v_d (high mobility), high w
- For fast switching we need high v_d (high mobility), small w
- For miniaturization we need small w, d_{ox}, A
- For small leakage we need high w, high d_{ox}

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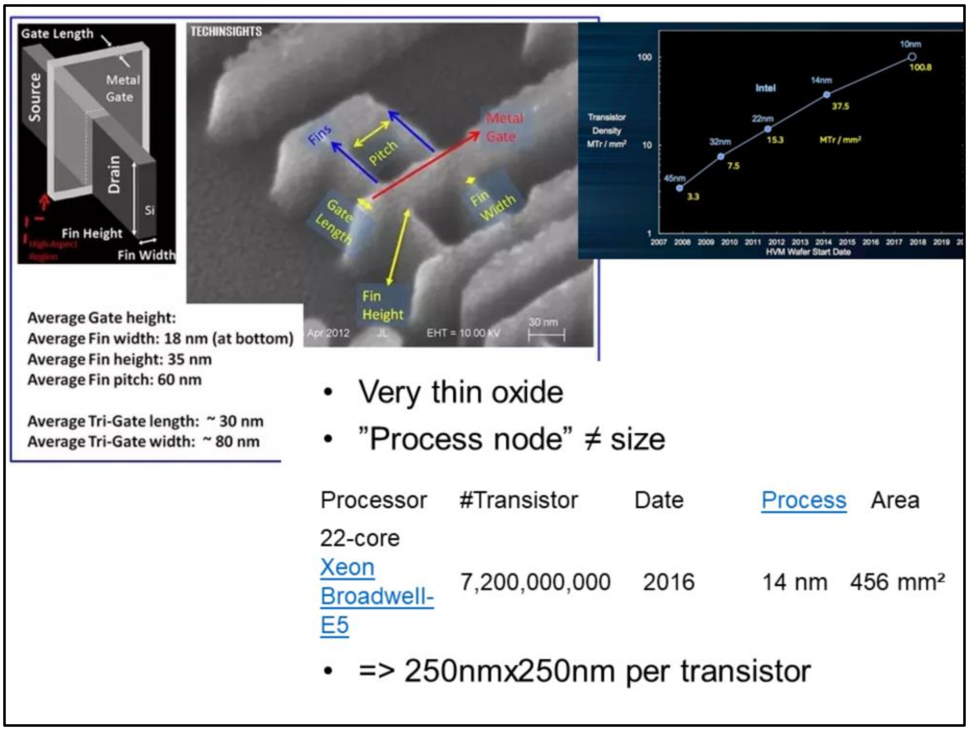
- Miniaturization (decreasing dimensions) lead to lower losses and thus less power consumption up to a point (where leakage starts to become unavoidable)



Average Gate height:
Average Fin width: 18 nm (at bottom)
Average Fin height: 35 nm
Average Fin pitch: 60 nm

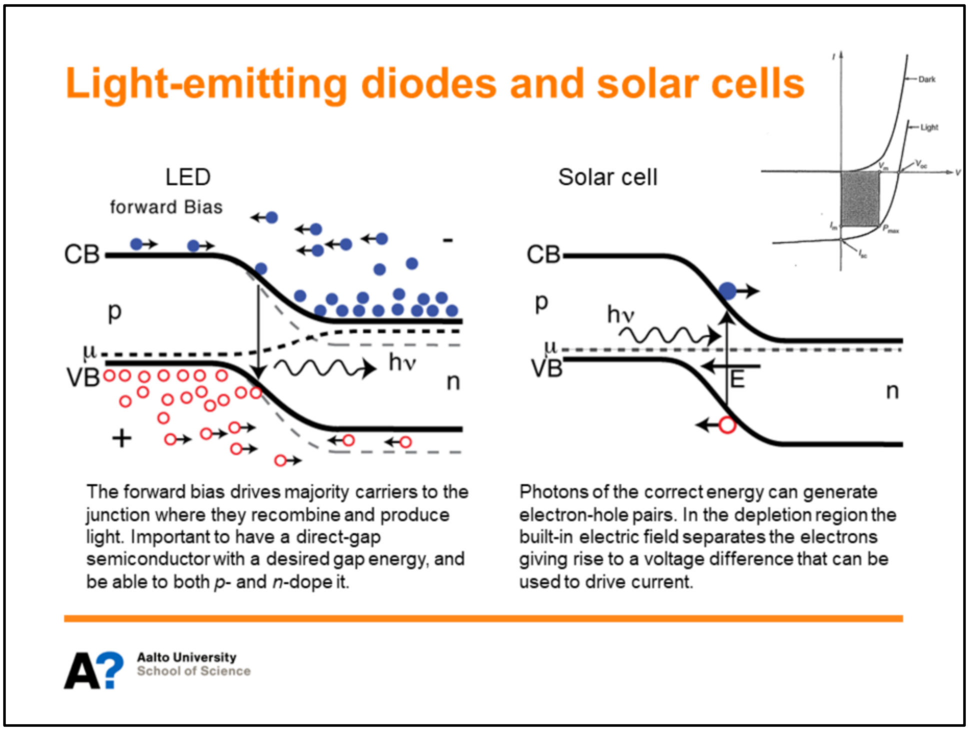
Average Tri-Gate length: ~ 30 nm
Average Tri-Gate width: ~ 80 nm

- Very thin oxide
- ”Process node” ≠ size

Processor	#Transistor	Date	Process	Area
22-core Xeon Broadwell-E5	7,200,000,000	2016	14 nm	456 mm²

- => 250nmx250nm per transistor

- Finfet design to increase width without increasing area on die.
- sqrt(456/7.2e9)= 2.5e-4, so 250nmx250nm per transistor on average. Size of one transistor will be smaller.
- Sqrt(2) decrease in process node still translates to roughly doubling of transistor density.
- Oxide thickness is getting close to atomic-scale limits



Light-emitting diodes and solar cells

The forward bias drives majority carriers to the junction where they recombine and produce light. Important to have a direct-gap semiconductor with a desired gap energy, and be able to both *p*- and *n*-dope it.

Photons of the correct energy can generate electron-hole pairs. In the depletion region the built-in electric field separates the electrons giving rise to a voltage difference that can be used to drive current.

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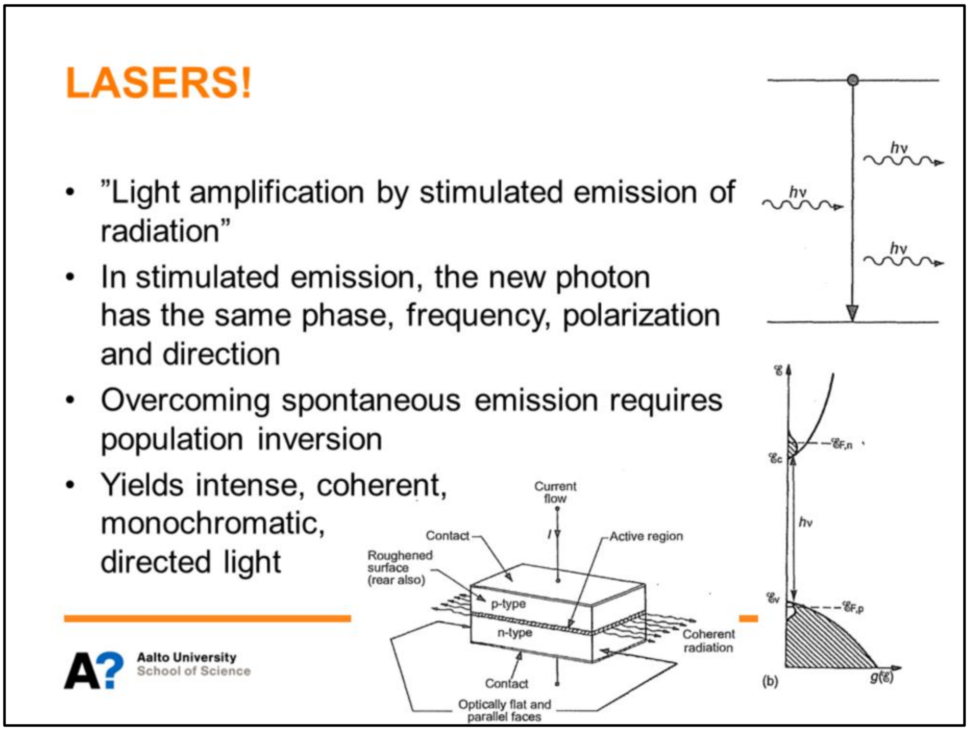
- As alluded about GaN, the achievements resulting in nobel: able to grow good quality GaN (and AlGaN) and p-type dope it.
- Illumination increases the drift current. Possible to extract work under forward bias.



LASERS!

- ”Light amplification by stimulated emission of radiation”
- In stimulated emission, the new photon has the same phase, frequency, polarization and direction
- Overcoming spontaneous emission requires population inversion
- Yields intense, coherent, monochromatic, directed light

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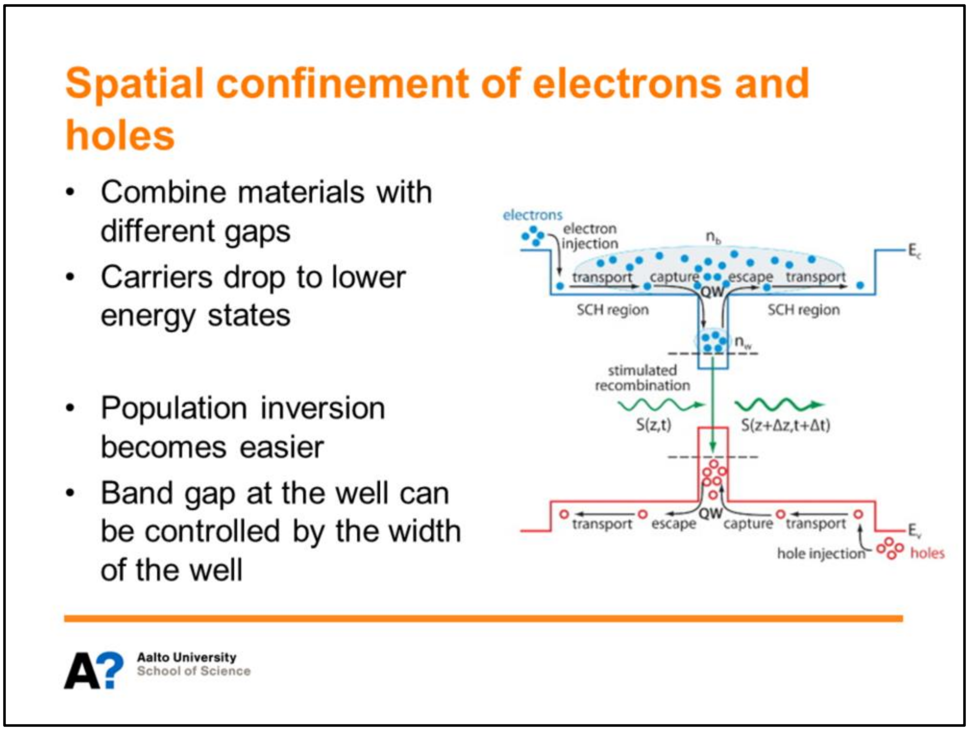
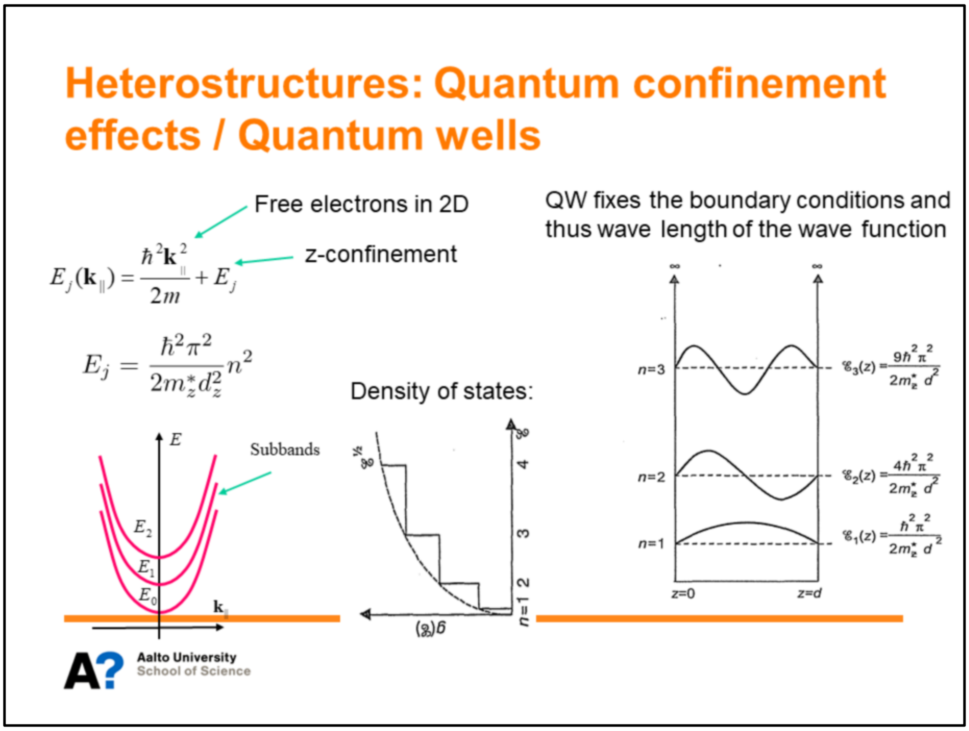
- Population inversion can be generated e.g. by pumping with higher energy photons or electrons from external circuit



Spatial confinement of electrons and holes

- Combine materials with different gaps
- Carriers drop to lower energy states
- Population inversion becomes easier
- Band gap at the well can be controlled by the width of the well

- Same idea both for LEDs and lasers



Heterostructures: Quantum confinement effects / Quantum wells

$$E_j(\mathbf{k}_{\|}) = \frac{\hbar^2 \mathbf{k}_{\|}^2}{2m} + E_j$$

Free electrons in 2D

z-confinement

$$E_j = \frac{\hbar^2 \pi^2}{2 m_z^* d_z^2} n^2$$

Density of states:

QW fixes the boundary conditions and thus wave length of the wave function

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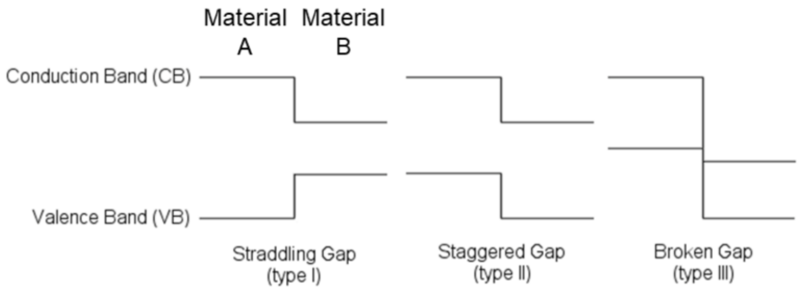
- The electrons are usually close to the valley minimum/maximum, thus the wave vector can be large (hundreds of Å). They are then sensitive to trying to force them in to a small potential well
- Schrödinger eq without cross terms: (H_xy + H_z)*psi(xy)*psi(z)= E*psi(xy)*psi(z),
- Electrons are free in lateral directions, plane wave solutions. Confined in z-direction, particle-in-a-box solutions
- States are pushed higher in energy

Different types of band alignments



Material A

Material B

Conduction Band (CB)

Valence Band (VB)

Straddling Gap (type I)

Staggered Gap (type II)

Broken Gap (type III)

How can one confine *i*) electrons, *ii*) holes or *iii*) both in the same well.

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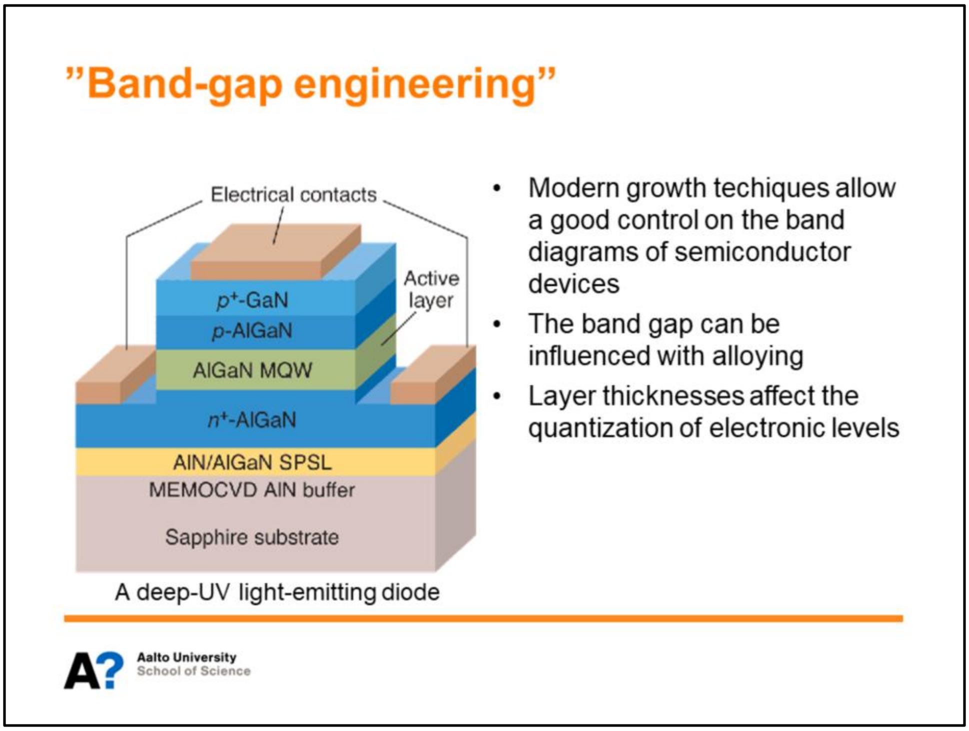

”Band-gap engineering”

A deep-UV light-emitting diode

- Modern growth techiques allow a good control on the band diagrams of semiconductor devices
- The band gap can be influenced with alloying
- Layer thicknesses affect the quantization of electronic levels

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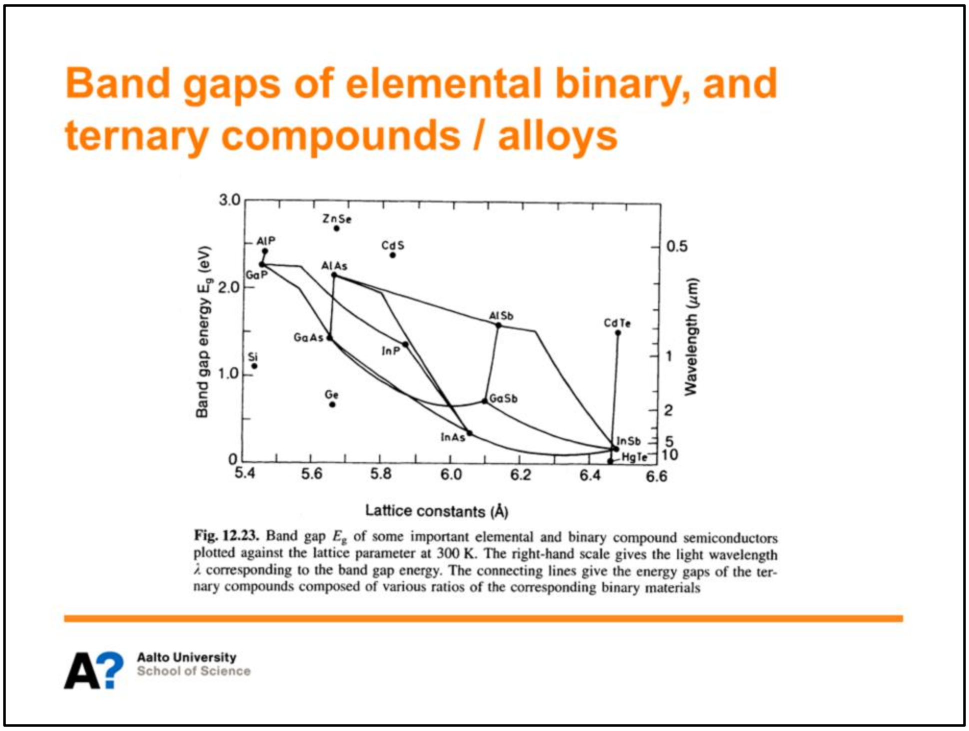
- SPSL: Short period superlattice,



Band gaps of elemental binary, and ternary compounds / alloys

Fig. 12.23. Band gap E_g of some important elemental and binary compound semiconductors plotted against the lattice parameter at 300 K. The right-hand scale gives the light wavelength λ corresponding to the band gap energy. The connecting lines give the energy gaps of the ternary compounds composed of various ratios of the corresponding binary materials

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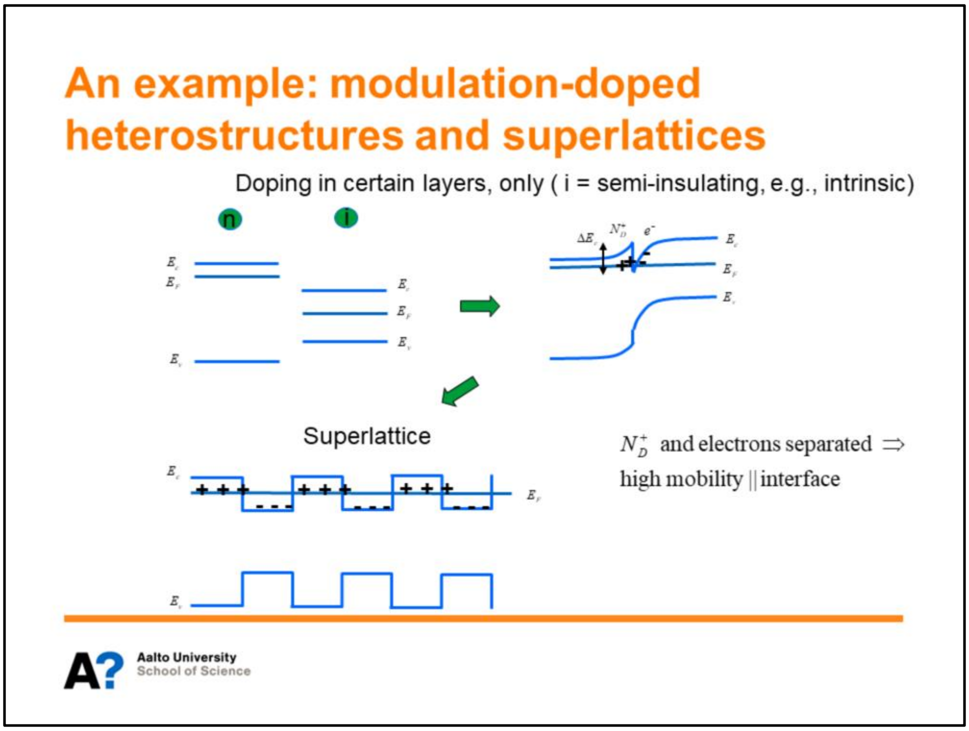
- Changing band gap (via alloying) also changes the valence band and conduction band minima positions and thereby band offsets



An example: modulation-doped heterostructures and superlattices

Doping in certain layers, only (i = semi-insulating, e.g., intrinsic)

Superlattice

N_D^+ and electrons separated $\Rightarrow$ high mobility || interface

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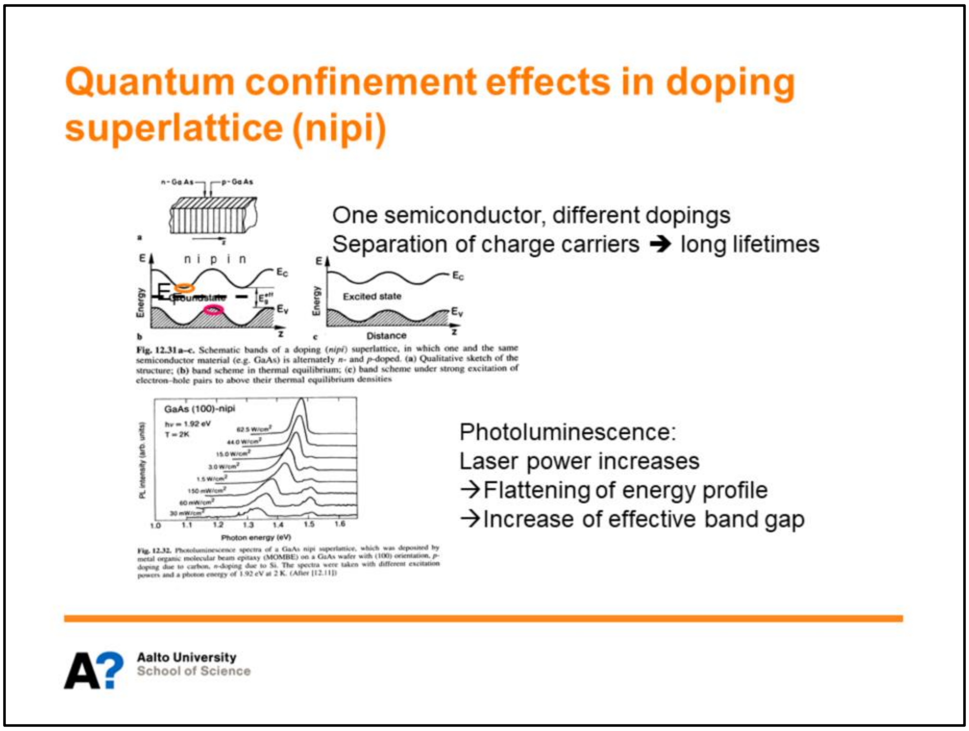
- Skip?



Quantum confinement effects in doping superlattice (nipi)

One semiconductor, different dopings

Separation of charge carriers ➔ long lifetimes

Fig. 12.31 a–c. Schematic bands of a doping (*nipi*) superlattice, in which one and the same semiconductor material (e.g. GaAs) is alternately *n*- and *p*-doped. (**a**) Qualitative sketch of the structure; (**b**) band scheme in thermal equilibrium; (**c**) band scheme under strong excitation of electron–hole pairs to above their thermal equilibrium densities

Photoluminescence:

Laser power increases

→Flattening of energy profile

→Increase of effective band gap

Fig. 12.32. Photoluminescence spectra of a GaAs nipi superlattice, which was deposited by metal organic molecular beam epitaxy (MOMBE) on a GaAs wafer with (100) orientation, *p*-doping due to carbon, *n*-doping due to Si. The spectra were taken with different excitation powers and a photon energy of 1.92 eV at 2 K. (After [12.11])

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Heterostructures and devices – summary in form of questions

1. Formation of the p-n junction or Schottky barrier. How does it function as a rectifier? What types of currents pass over the junction.
2. What are band offsets and band bending in heterostructures? On which properties do they depend on?
3. What type of effects does quantum confinement cause in heterostructures?
4. How does a MOSFET operate?
5. What are the main operating principles of LEDs and solar cells?

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This week's exercises and next week's topic

- Exercises of Friday: A more qualitative treatment of the Schottky model for the *p-n* junction (important also from the conceptual point of view)
- Next Monday: Defects (Elliott Chapter 3)

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