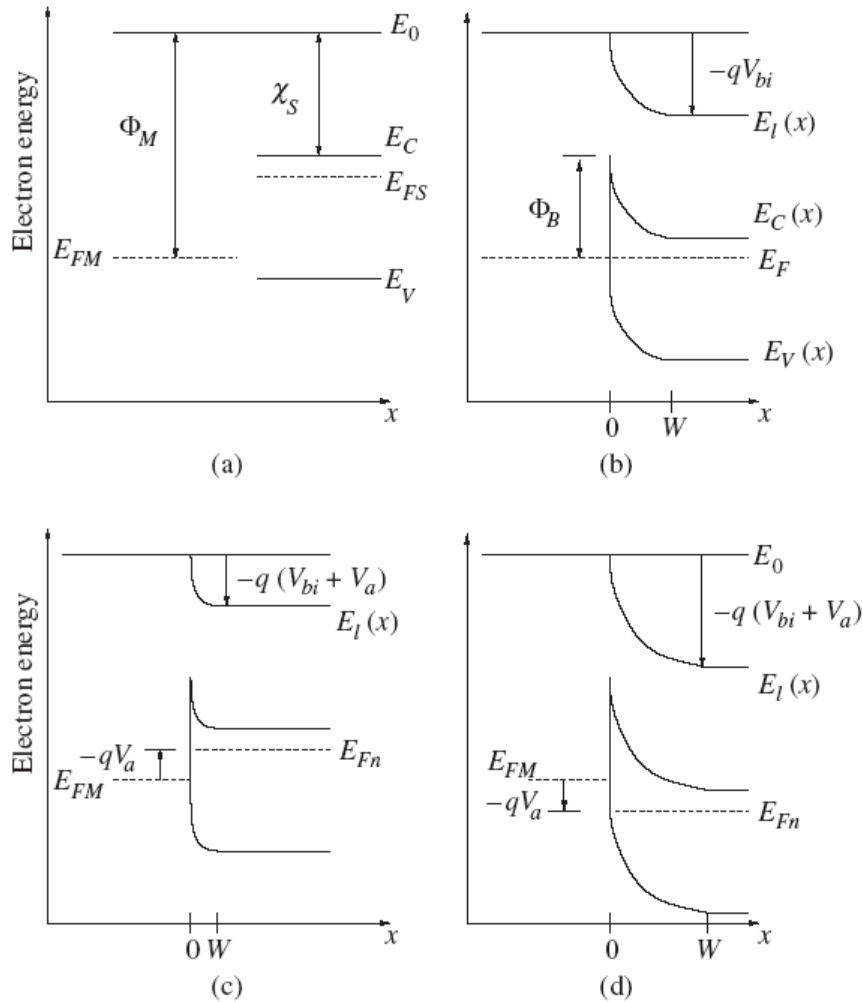


# Real heterojunctions

## LECTURE 9

- Schottky barrier current
- CdS/CIGS
- Energy band alignment “rules”
- CdTe/Ge
- Surface reconstruction, dipoles
- Surface states
- Fermi-level pinning

# HJ1: Schottky barrier

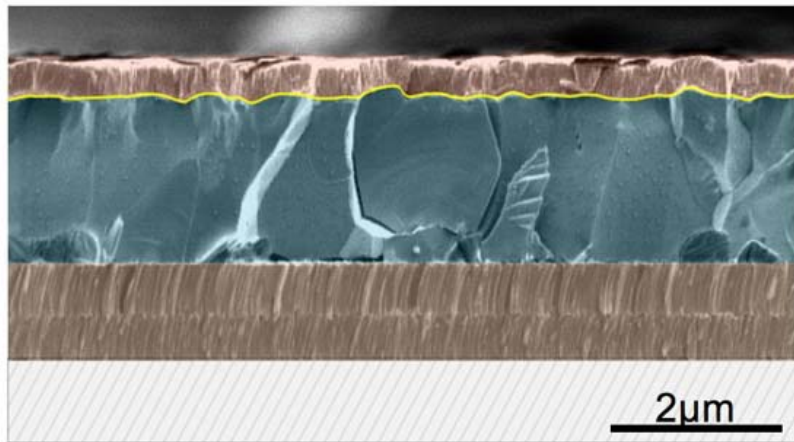


- Note discontinuity in Fermi level
- What is the forward-bias current?

**Figure 11.3** Energy-band diagrams showing a metal/semiconductor junction. (a) Prior to joining the two components. (b) At equilibrium. (c) Forward bias. (d) Reverse bias.

## Sec. 7.6.1

# Heterostructure, thin film, cells: a lower cost alternative (?)



ZnO/CdS

CIGS

Mo

Glass

## CIGS

ZnO, ITO - 2500 Å

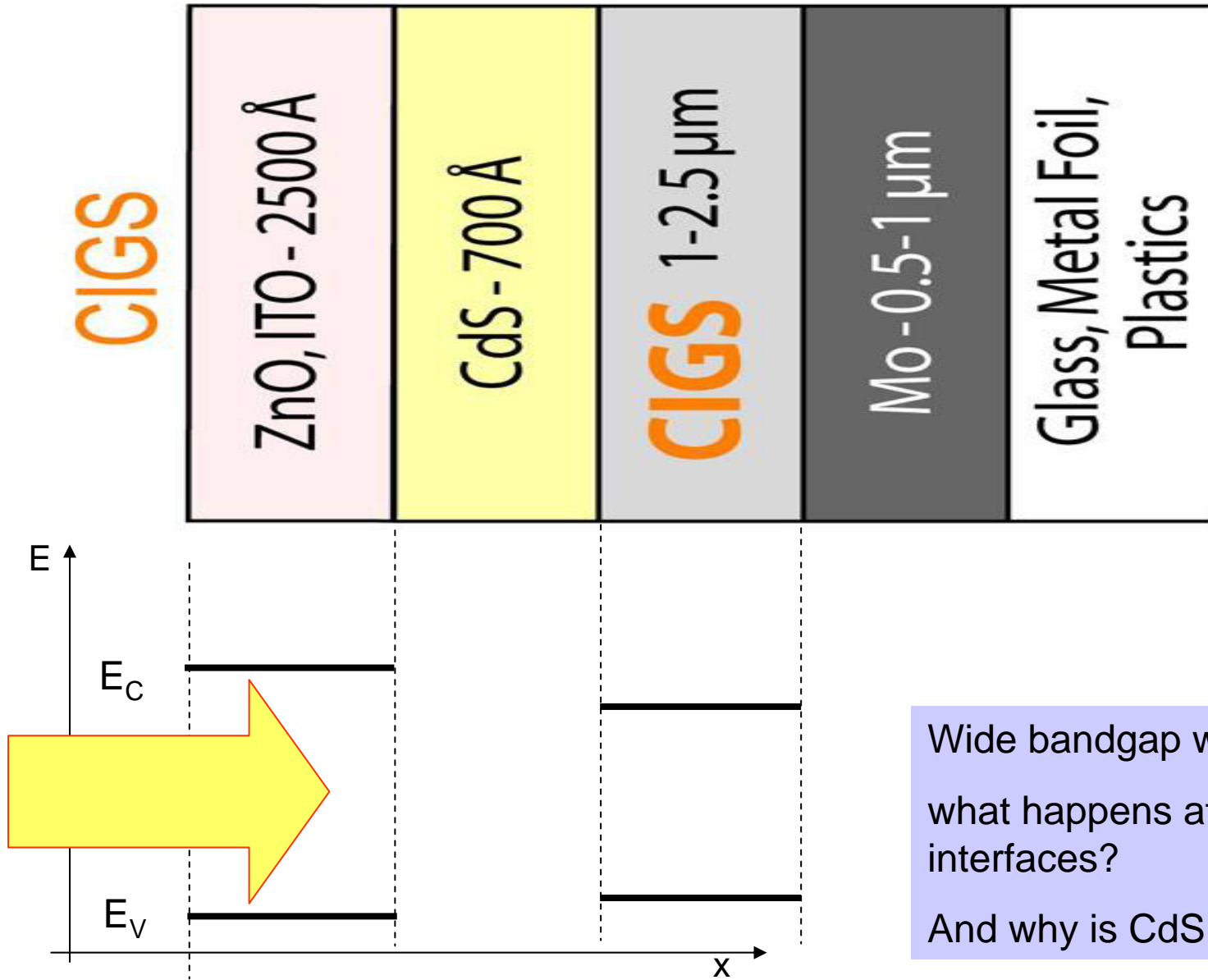
CdS - 700 Å

**CIGS** 1-2.5 μm

Mo - 0.5-1 μm

Glass, Metal Foil,  
Plastics

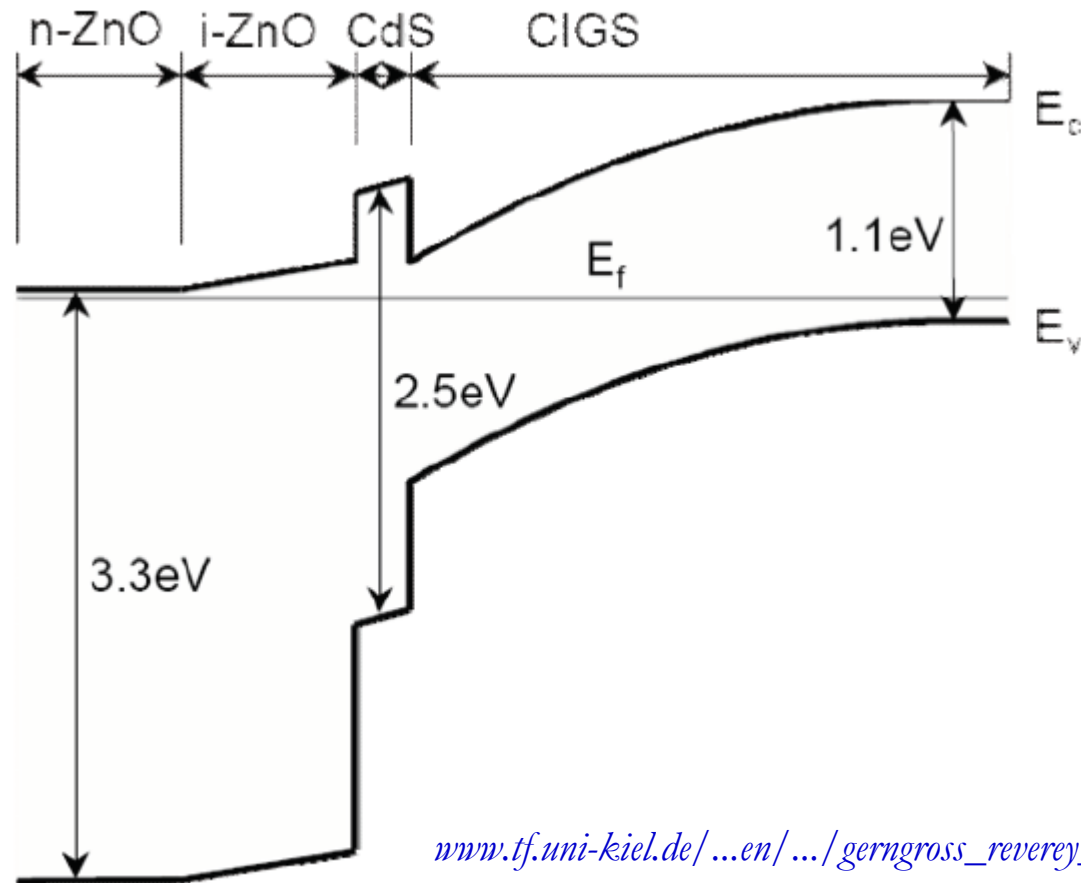
## HJ2: CdS/CIGS



Wide bandgap window, but what happens at the interfaces?

And why is CdS needed?

# A proposed band diagram

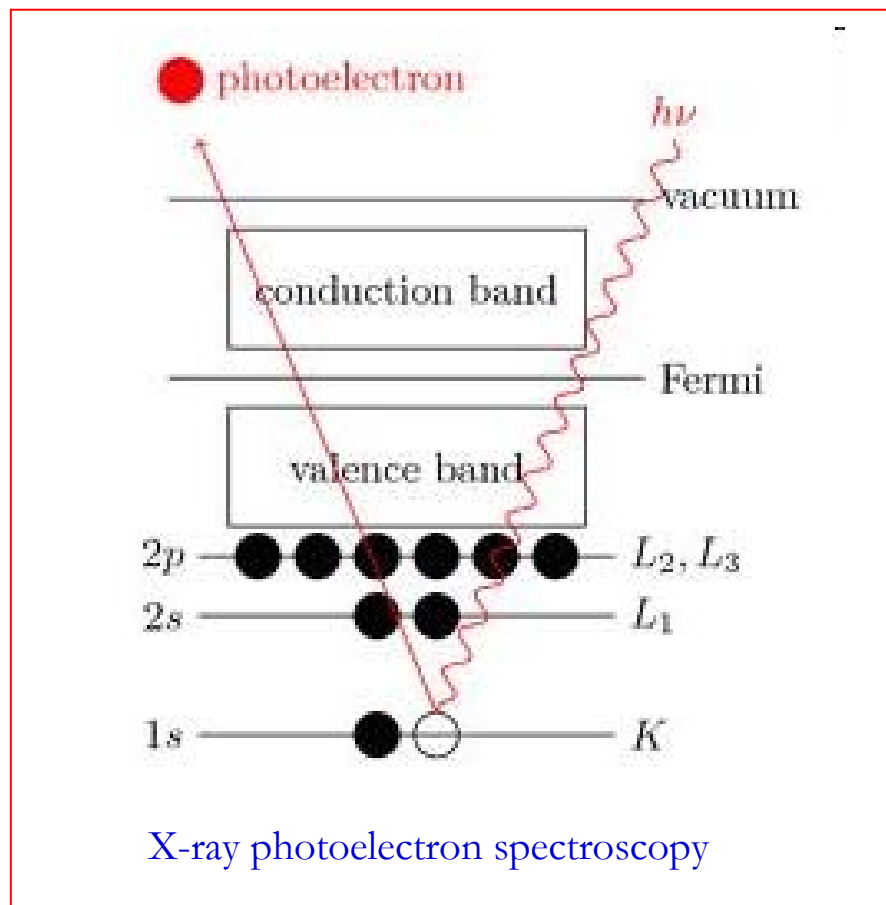


**Figure 5:** Band-gap structure of ZnO/CdS/CIGS module

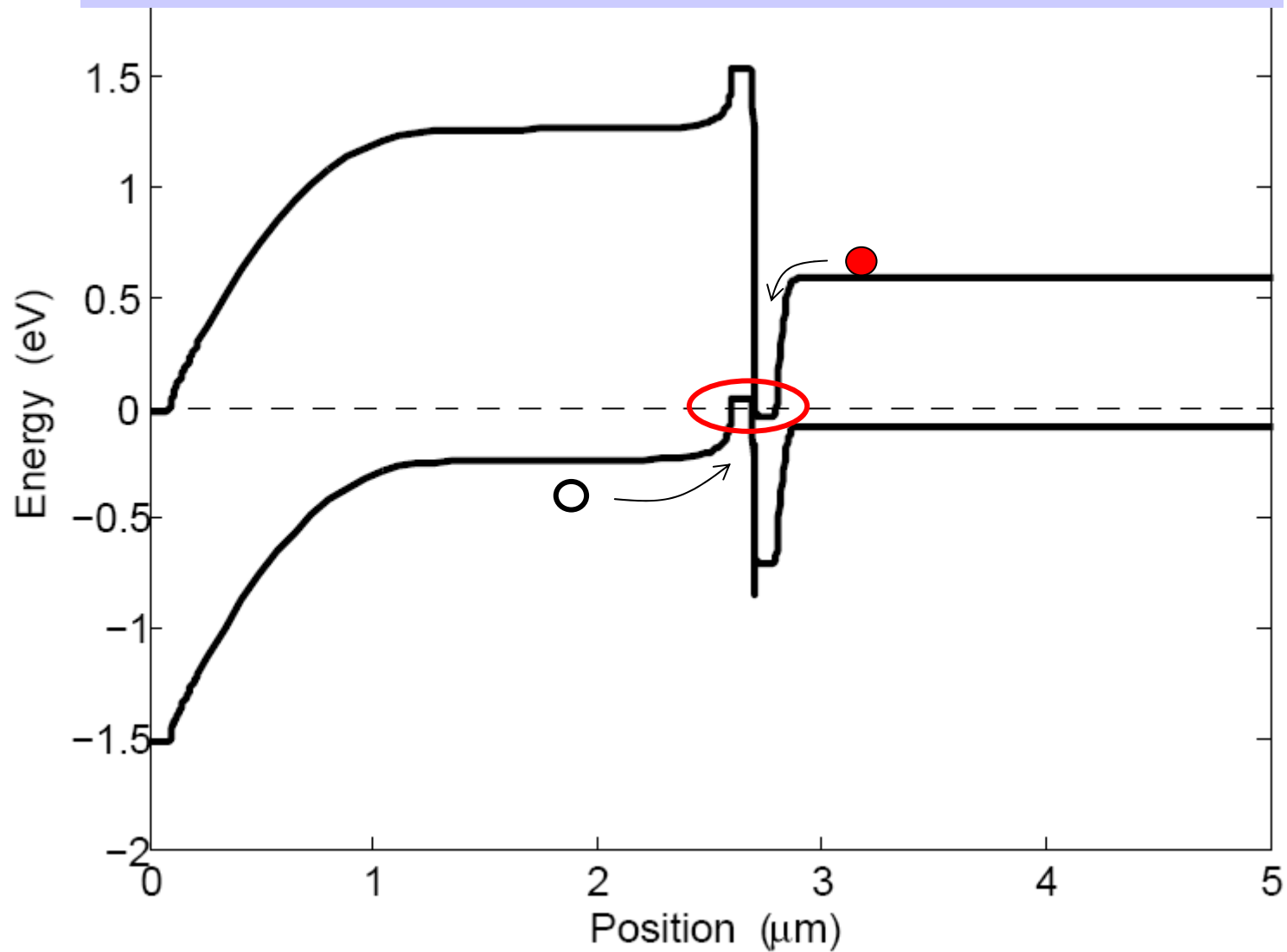
How was the band alignment determined?

# Band alignment

1. Anderson Rule: alignment via electron affinities.
2. “Kroemer Rule”: alignment via valence-band offset.



## HJ3: Band discontinuity at CdTe/Ge interface



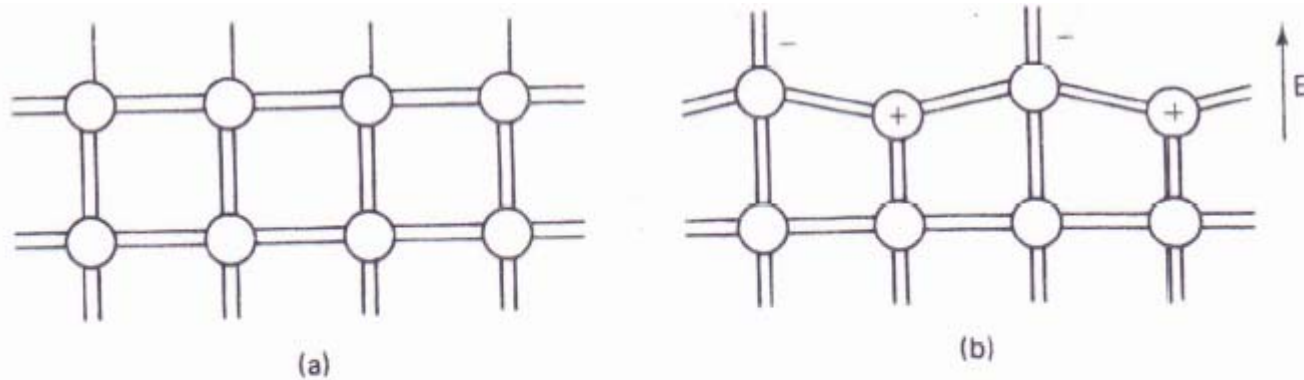
# Real heterostructures

Some practical factors affecting band alignment:

- surface reconstruction
- dipole formation
- interruption of the periodicity of the semiconductor
- surface states



# Surface reconstruction

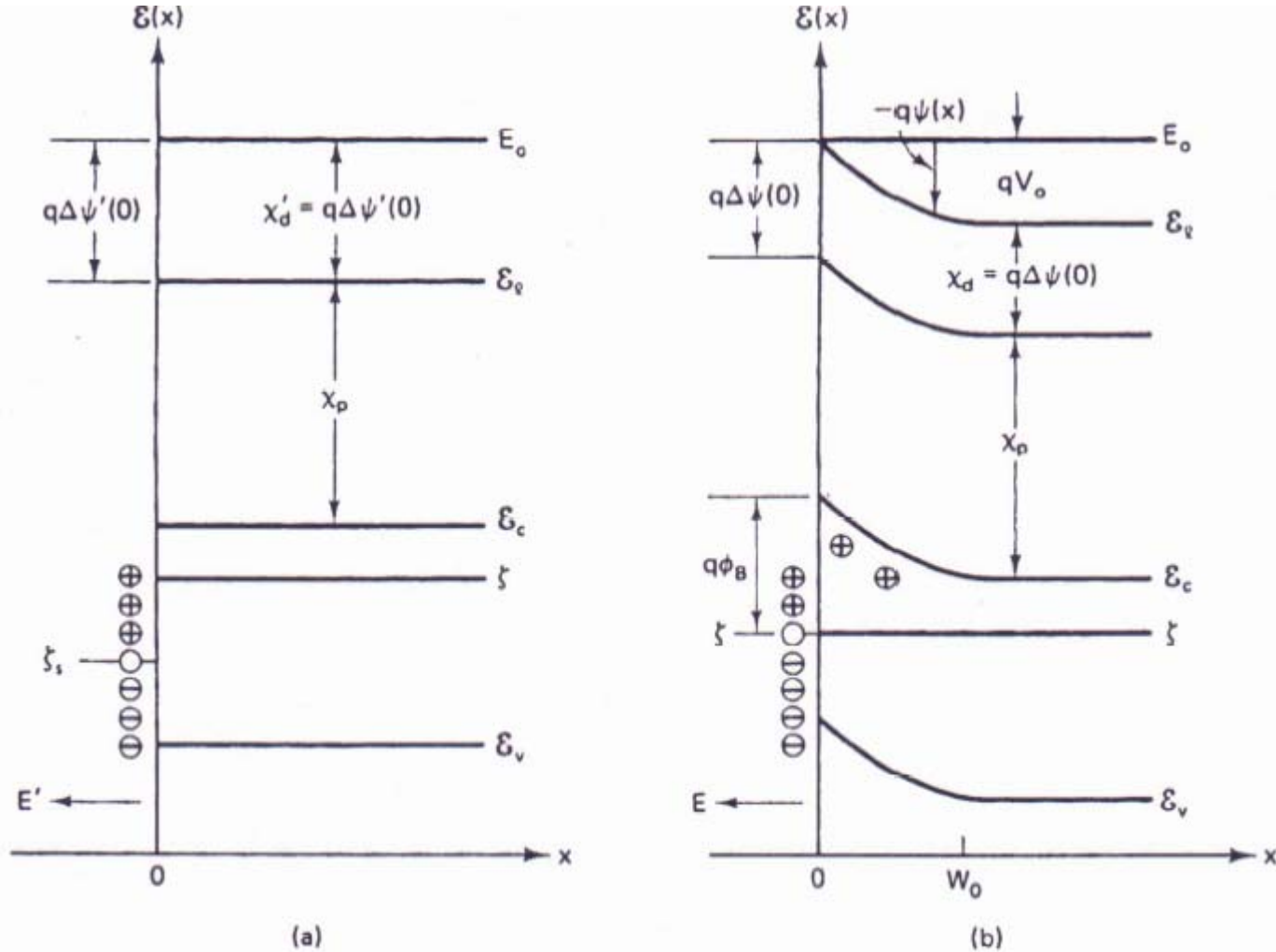


**Figure 10.2** Schematic illustration of surface dipole formation. In (a) each neutral surface atom has one dangling bond. In (b) the dangling bonds pair and produce a shift in atomic positions.

What is the magnitude of the surface field?

How does it affect the band diagram?

# Effect of surface dipoles



**Figure 10.3** Effects of surface dipoles on energy band structure (a) before and (b) after charge transfer between the surface and the bulk material.

# Lattice mismatch

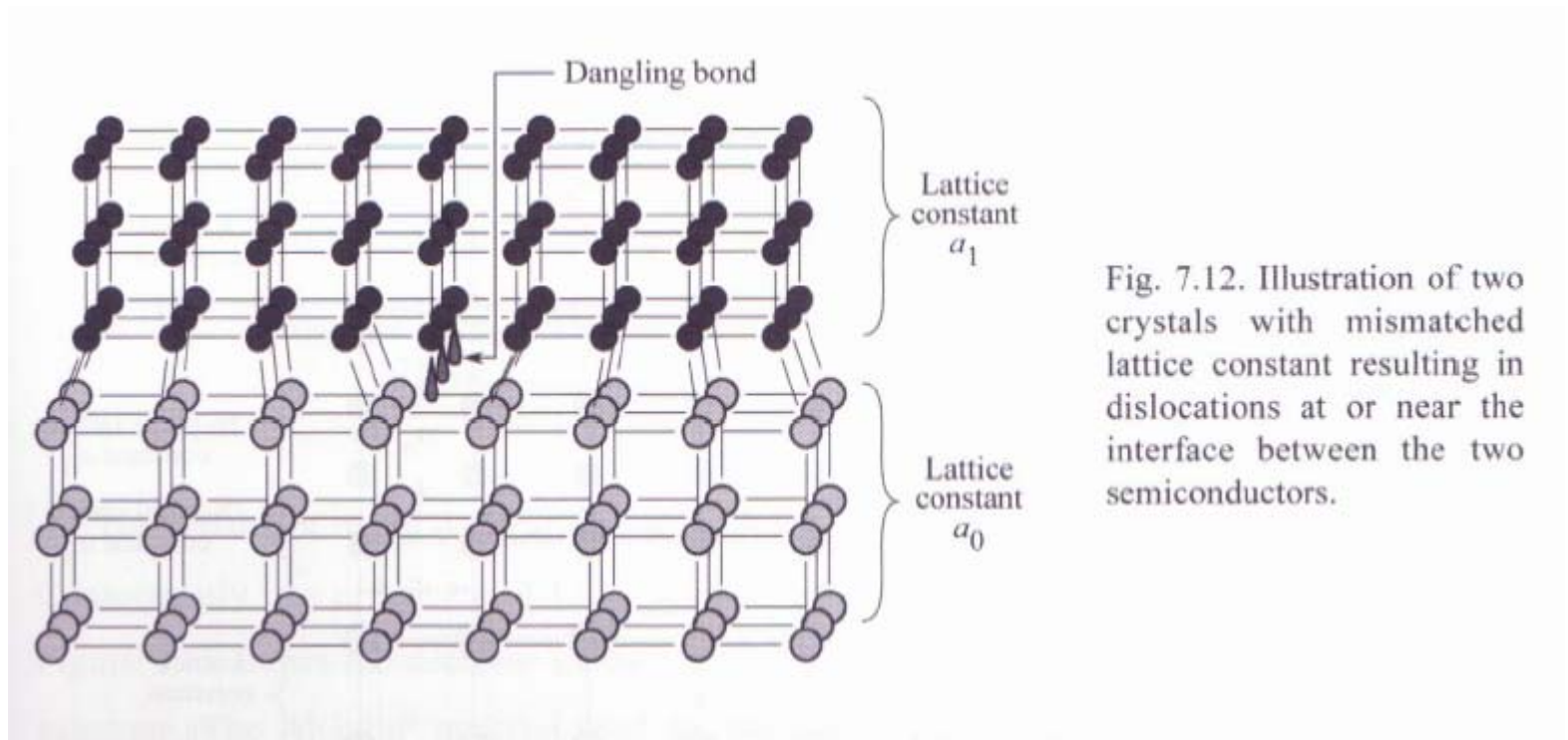
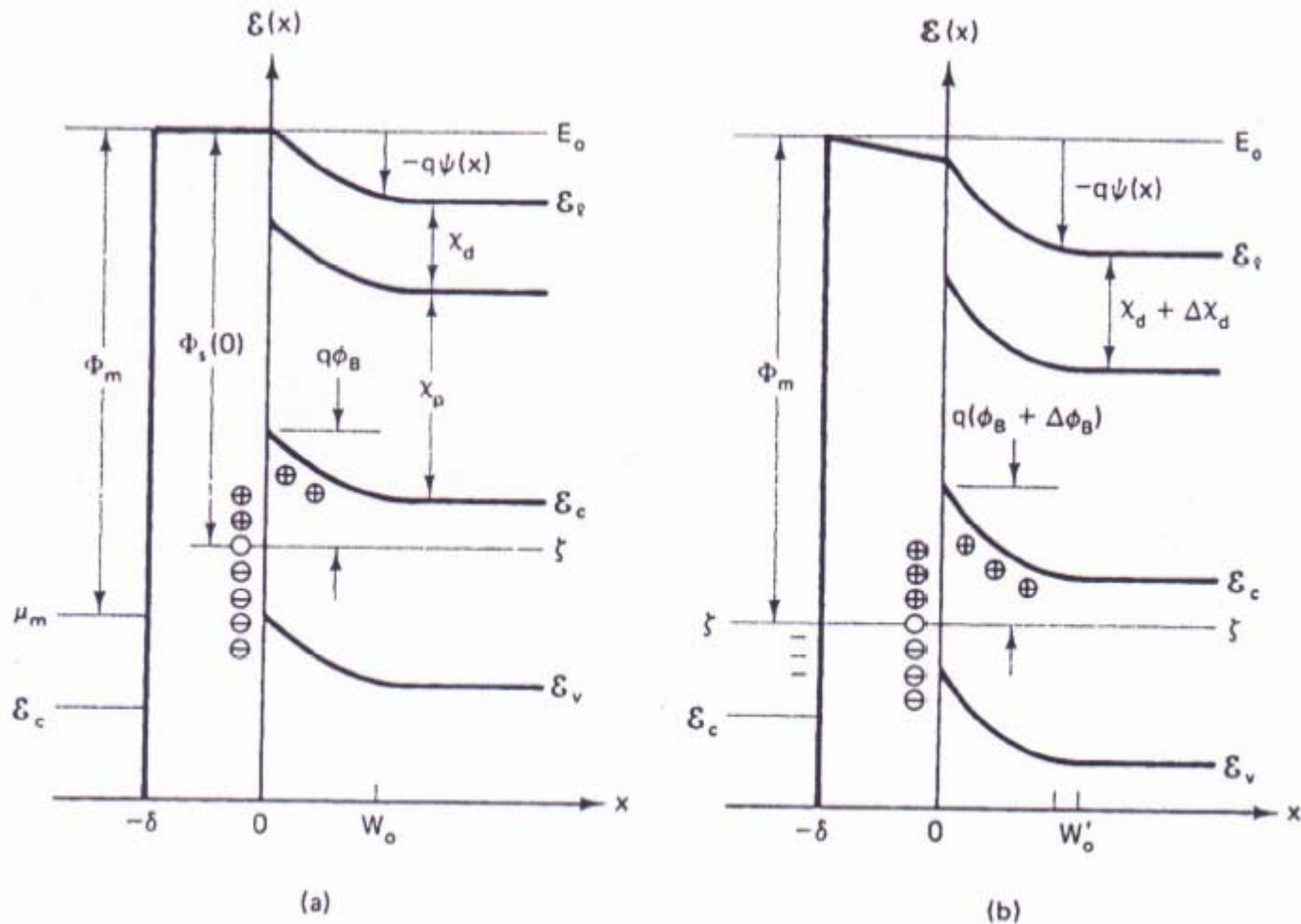


Fig. 7.12. Illustration of two crystals with mismatched lattice constant resulting in dislocations at or near the interface between the two semiconductors.

*E.F. Schubert, LEDs, CUP, 2007*

Dislocations cause intra-gap states, and non-radiative recombination.

# Effect of surface states



**Figure 10.6** Energy band diagrams of a metal–semiconductor pair with  $\Phi_m > \Phi_s$  and surface states (a) before and (b) after thermal equilibrium.