Photoemission models

Photoemission can be described with the *one-step model,* where the initial state consists of the photon and the electrons in the ground state. In the final state, after the photon absorption, the photoelectron is in an initially empty state outside of the solid.

An approximation to the above is the *three-step-model:*

1. Excitation of the electron to an empty conduction band state following the photon absorption.
2. Ballistic transport of the photoelectron to the surface.
3. Transmission of the photoelectron through the surface.

8.2. Inverse Photoemission

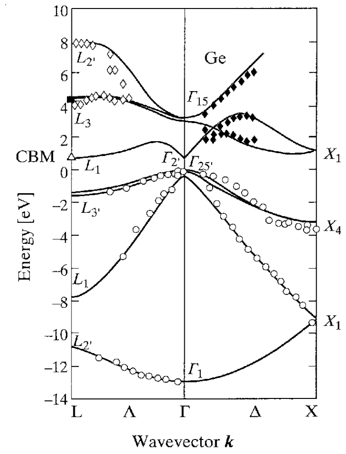


Fig. 8.23 Measured band structure of Ge.

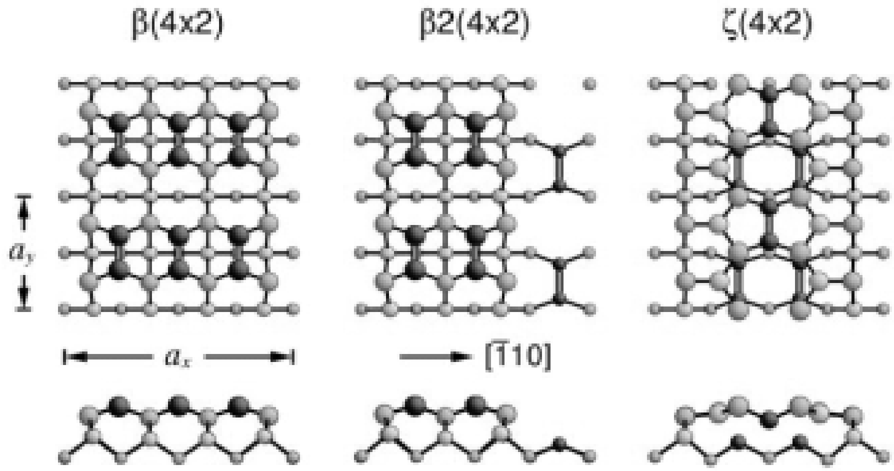
8.3. Surface Effects

Surfaces break the 3D periodicities and by that effect on the electronic structures, most clearly seen as new electronic states.

8.3.1. Surface States and Surface Reconstruction

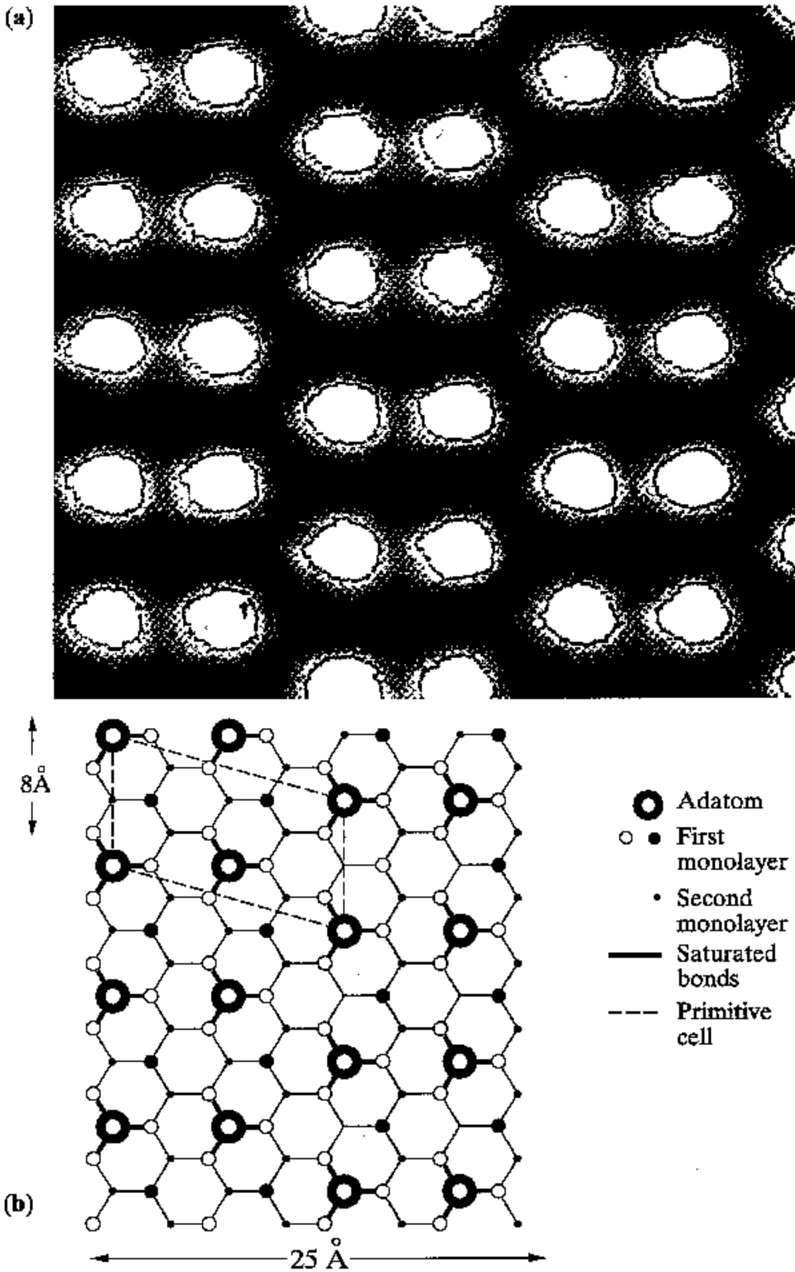
Cleaving the semiconductor and creating the surface breaks bonds and leaves signly occupied *dangling bonds* pointing out of the surface. These states form 2D bands, which may appear in the bulk band gap as surface states. If they, however, overlap in energy with bulk bands, they may broaden to surface resonances.

Unsaturated dangling bonds may also try to become saturated by *surface reconstruction.* This is analogous to *Peierls transition,* where a half-occupied (metallic) band splits to two: fully occupied and empty, by doubling the primitive cell size (bulk reconstruction).

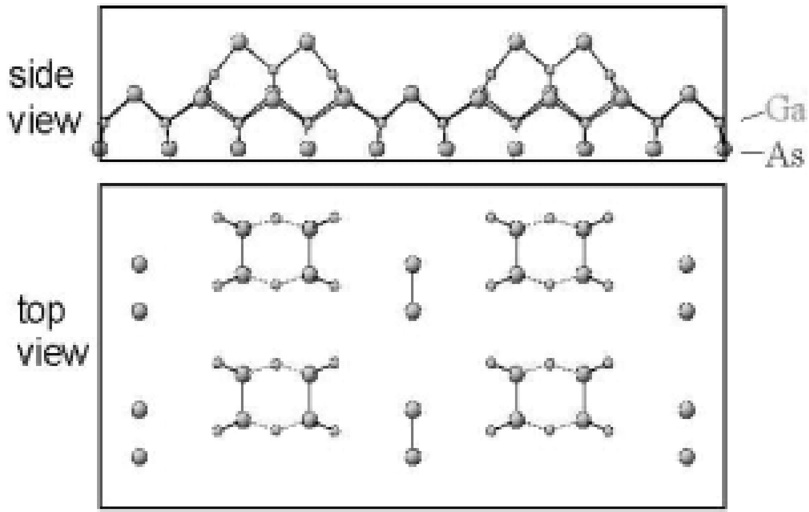


Some surface reconstructions of GaAs (001) surface

Surfaces can be studied by Scanning Tunneling Microscopy (STM), see Ge(111)-c(2x8) surface in Fig. 8.24, below.



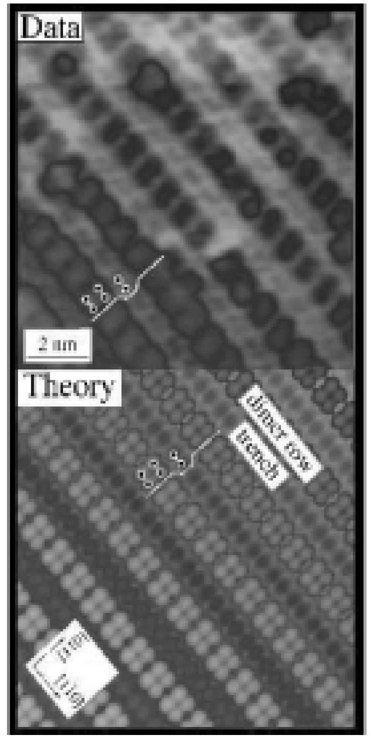
β2 reconstruction of GaAs (001) (2x4) unit cell



STM imaging of GaAs(001)

measured filled state image at V_{tip}= - 2.1eV →

simulated image local density of states integrated to 0.3 eV below the valence band maximum →



LaBella, Yang, Bullock, Thibado, Kratzer & Scheffler, PRL ***83****, 2989 (1999).*

8.3.2. Surface Energy Bands

As surfaces are periodic in two dimensions, only, the reciprocal space is two dimensional, too.

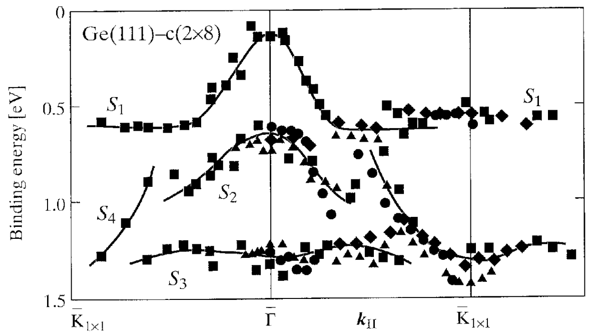
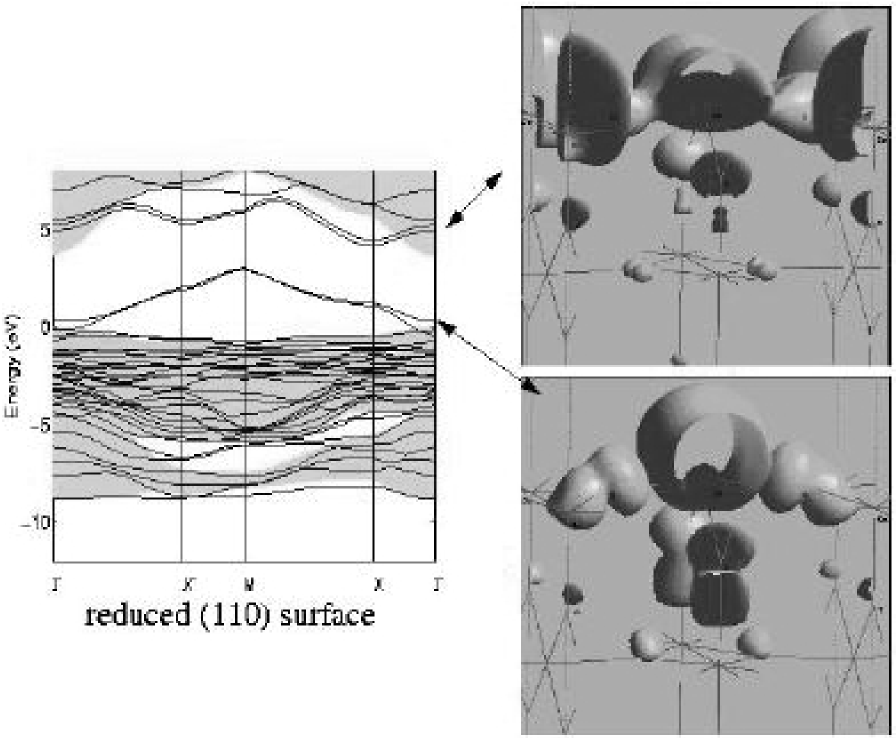


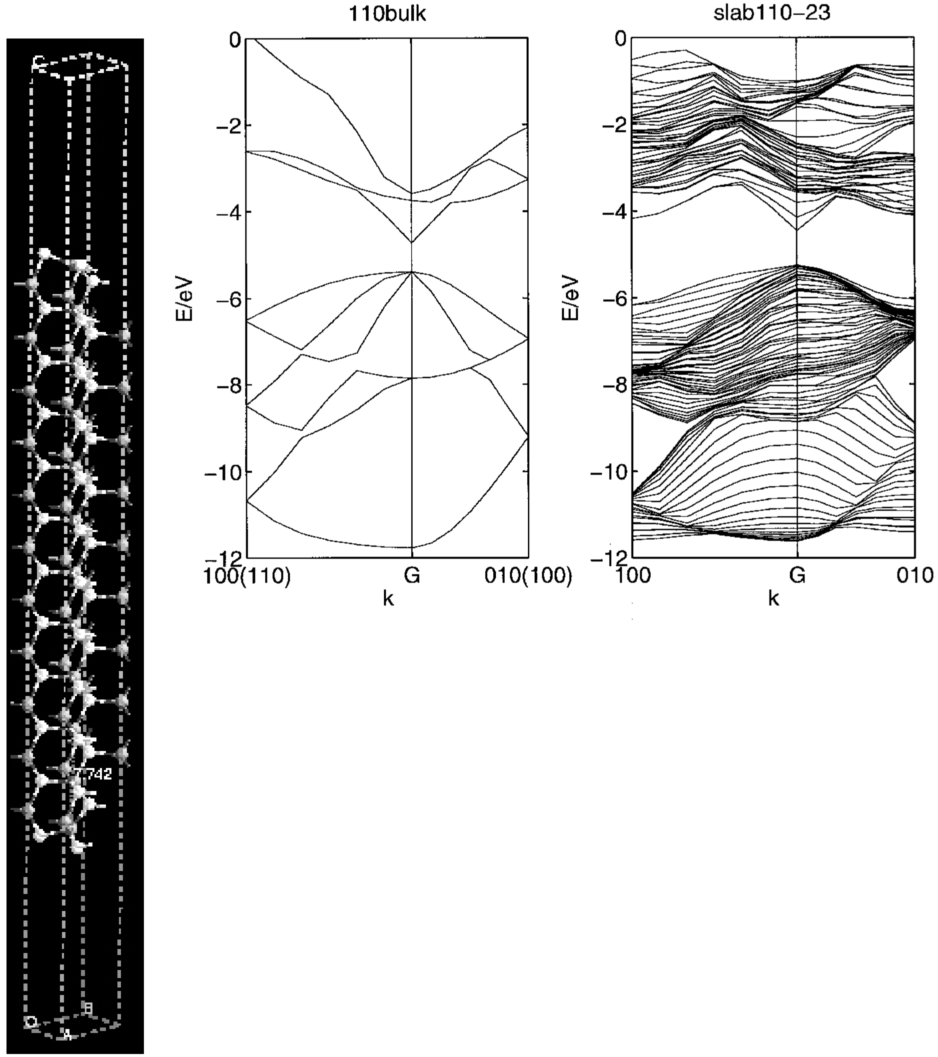
Fig. 8.25. Ge(111)-c(2x8) surface bands.

The three dimensional (3d) bulk bands can be projected from the 3D Brillouin zone onto the 2D surface Brillouin zone.

Fig. Reduced (110) surface bands of SnO_2. Bulk projection shown by green.



Bulk and surface bands of GaAs (110) obtained from DFT–LCAO calculation with a slab model.



Constant density surface of GaAs (110) surface illustrated by constant height curves as a simple model for STM picture.

<u>8.3.3. Fermi Level Pinning and Space Charge Layers</u>

The surface electronic states may or may not be in the band gap. If the surface bands are in the bulk band gap they are narrow compared to the surface bands overlapping the bulk bands and forming sc. *resonances.*

In the figure 8.27., below:
a) the bulk band gap is free of surface bands
b) p-type semiconductor with E_F pinning: hole depletion layer
c) n-type semiconductor with E_F pinning: electr. depletion layer
d) intrinsic semiconductor with E_F pinning: hole enrichment layer

9. Effects of Quantum Confinement

Quantum size confinement of charge carriers is achieved using various type of nano scale structures. The first one was the *superlattice* at 1970's. Others are the *quantum wells* (QW), *quantum wires* and *quantum dots* (QD).

In fabrication of nano structures atomic level accuracy is desirable. It can be achieved by MBE of MOCVD. Also self-organization.

Surface diffusion, growth, and self-assembly of quantum dots at III-V semiconductor surfaces

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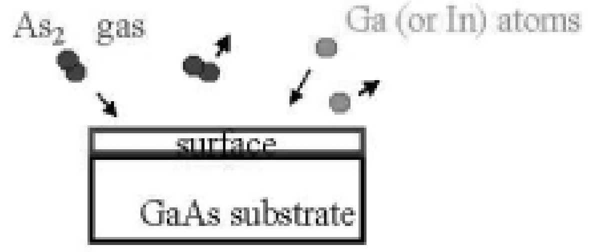
http://www.fhi-berlin.mpg.de/th/th.html

Microscopic processes controlling the growth of III-V semiconductors



1) deposition of Ga and As
2) adsorption of Ga
3) diffusion of Ga
4) desorption of Ga
5) adsorption of As_2 ?
6) dissociation of As_2 ?
7) diffusion of As
8) desorption of As
9) island nucleation
10) growth

key investigator: Peter Kratzer