A theoretical investigation of photoemission spectra from $(GaAs)_m(AlAs)_n$ superlattices

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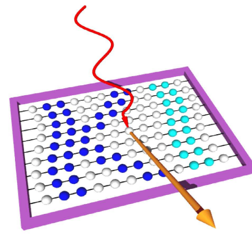


Introduction

Superlattices, formed by ultrathin layers of different semiconductor materials, cannot be treated as being composed of layers with their individual band structures. On the contrary, the electronic properties are determined by the entire superlattice as a whole. The larger periodicity perpendicular to the surface changes the symmetry of the Brillouin zone. This results in a back folding of the valence bands of the bulk material, which opens additional gaps at the edges of the Brillouin zone.

We present theoretical photoemisison spectra for $(GaAs)_2(AlAs)_2$ and $(GaAs)_3(AlAs)_3$ superlattices in the (001) orientation. The spectra are calculated in the one-step model, explicitly including the sequence of semiconductors in the initial states as well as in the final states and the matrix elements.

The theoretical investigation shows, that angle resolved normal emission photoelectron spectroscopy is capable to detect the period of the lattice by specific gaps.

The detailed analysis of the origin of emissions reveals that excitations even below the third layer are accessible and clearly distinguishable by photoemission.

Accurate numerical one-step calculations are required for a successful interpretation of such experimental data.

Numerical Details:

- one-step model

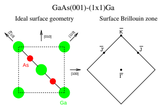
Initial states:

- LCAO
- Half space Green's function

Final states:

- empirical pseudopotentials (K.A. Mäder and A. Zunger, Phys. Rev. B 50, 17393 (1994))
- time reversed LEED state

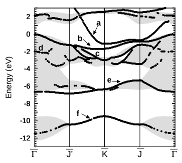
Surface geometry and surface Brillouin zone for the (001) surface



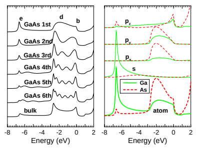
URL: http://www.tp.cau.de/schattke/

GaAs(001)-(1x1)Ga

Surface band structure

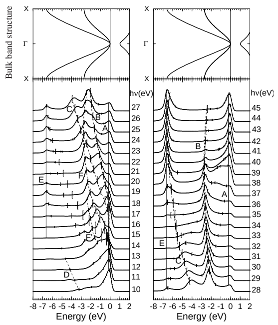


Density of states at $\bar{\Gamma}$



a) Ga p_x bridge bond state
b) Ga and As p_z dangling bond state
e) Ga s surface state

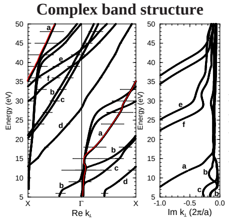
Normal emission spectra



Spectra in normal emission. Bars indicate binding energies at which direct transitions would be expected.

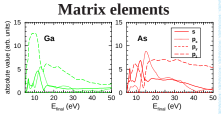
A) Emission from the Ga and As p_z dangling bond state (compare with the matrix elements below) , for photon energies above 33 eV also direct transitions
B,C,D,E,F,F') Direct transitions, especially B and C to final state a) (see the complex band structure below)
E) Emission from the Ga s surface state, for photon energies above 37 eV also direct transitions

Complex band structure



Complex band structure of GaAs(001). Bars indicate the magnitude of the expansion coefficients of the final state with respect to the complex bulk bands.

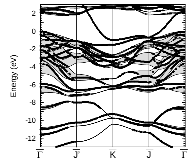
Matrix elements



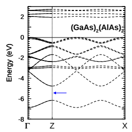
Modulus of the matrix elements of the two uppermost atomic layers of the GaAs(001)-(1x1)Ga surface resolved into orbitals

$(AlAs)_2(GaAs)_2(001)$-(1x1)Ga

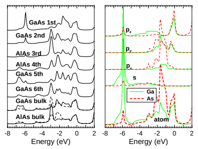
Surface band structure



Bulk band structure

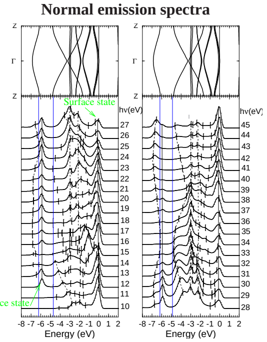


Density of states at $\bar{\Gamma}$

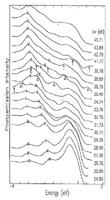


For the superlattice the symmetry of the Brillouin zone changes from face-centered cubic for GaAs and AlAs to a tetragonal one. The resulting band structure can be understood by back folding of the bulk valence bands into the smaller Brillouin zone, together with the opening of band gaps at their edges (see for example the blue arrow in the bulk band structure.

Normal emission spectra



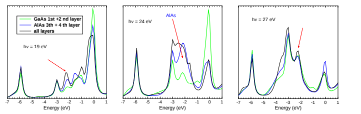
Experimental spectra Normal emission



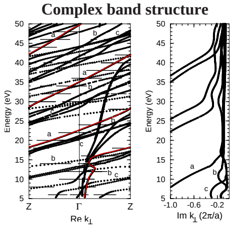
(Cai et al., Phys. Rev. B **46**, 6891 (1992))

The photoemission spectra reproduce the opening of the gap around -6.0 eV which is a characteristic property of the superlattice.

Layer resolved photocurrent

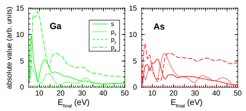


Complex band structure



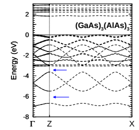
The layer resolved photocurrent shows, that for excitation energies between 21.0 and 25.0 eV the main contributions to the photocurrent at -2.0 eV is related to emissions from the AlAs layers which are below the first two GaAs layers.

Matrix elements

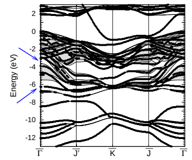


$(AlAs)_3(GaAs)_3(001)$-(1x1)Ga

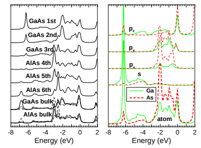
Bulk band structure



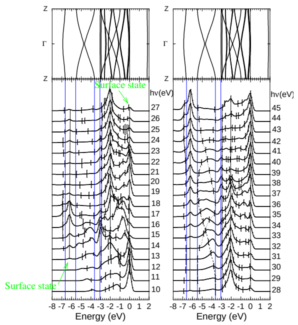
Surface band structure



Density of states at $\bar{\Gamma}$



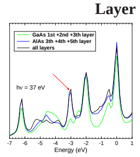
Normal emission spectra



The addition of one more layer GaAs and AlAs respectively generates an additional gap near -3.4 eV (blue arrow)

The normal emission spectra of $(AlAs)_3(GaAs)_3(001)$-(1x1)Ga show the additional band gap near -3.4 eV.

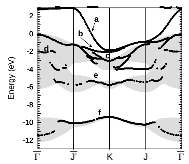
Layer resolved photocurrent



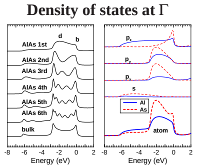
For the structure at -3.0 eV emissions from the AlAs layers below the first three GaAs layers are found

AlAs(001)-(1x1)Al

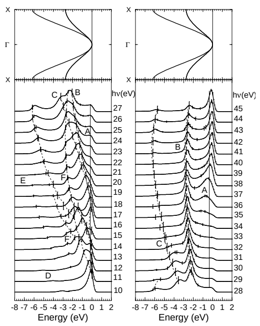
Surface band structure



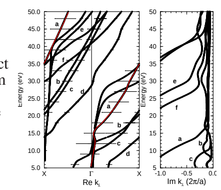
Density of states at $\bar{\Gamma}$



Normal emission spectra



Complex band structure



As for the GaAs(001) surface also from AlAs(001) strong direct transition could be expected from theory.
The emissions for GaAs near the lower valence band edge are missing for AlAs.