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AZIMUTHAL DEPENDENCE OF GAAS(110) ULTRAVIOLET PHOTOEMISSION SPECTRA

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The results of a new theoretical determination of the valence band photoemission spectra for the GaAs(110) surface are presented and compared with new experimental data. In discussing the azimuthal angular dependence of the spectra we focus on symmetry and topological properties of the polar plots. The calculations are carried out within the most elaborate technique, i.e. by using the one-step model. The orbital compositions of the structural features as well as their relative intensities are investigated. As compared to a rotation of the sample, here the sample is kept fixed during the computer controlled rotation of the electron analyser in the experiment. This allows not only to consider the variation with emission angle but also to study the influence of different directions of light.

Valence band photoemission spectroscopy usually detects the current for emission angles and corresponding k-values on high symmetry lines of the reciprocal space. On the other hand, photoelectron diffraction considers the emission into the full hemisphere and therefore probes not only the polar but also the azimuthal dependence. To take advantage of such additional information and to proceed towards a common understanding of both methods, we investigate azimuthal scans of the UV-photoemission of GaAs(110). We focus here on the investigation of the dangling bond state. As a surface state it is well separated from bulk states for the considered energies and k-values, thus simplifying the interpretation of the data.

The surface band structure, the surface density of states (SDOS), and the initial states of the photoemission are calculated in a layer orbital LCAO basis. The Hamilton matrix for the halfspace is determined with the extended Hückel theory [1] and the Green's matrix is computed [2]. The Green's matrix provides a description of the valence states and of the electronic structure via

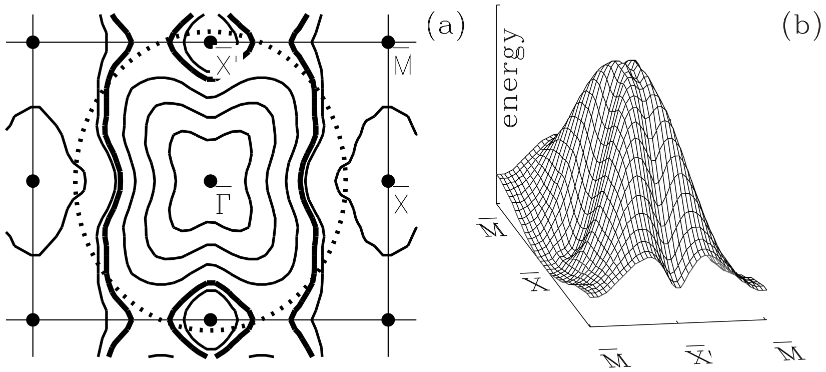

Figure 1: Structure of the dangling bond band: (a) contour plot of several energy levels of the band, together with high symmetry points, the circle of k-values for the discussed current (dotted), and the level for -0.75 eV (thick); (b) perspective view of the band.

the SDOS. We focus on the dangling bond band, which is shown in Fig. 1. It disperses from -0.08 eV in $\overline{\Gamma}$ to -1.07 eV, -0.9 eV, and -0.92 eV in $\overline{X}$, $\overline{X'}$, and $\overline{M}$, respectively. In Fig. 1a the contour plot and in Fig. 1b the perspective view of the dangling bond band show clearly its anisotropy, which extends over the whole Brillouin zone. With the z-direction pointing into the vacuum and the y-direction in the mirror plane, the p_y- and p_z-orbitals are the main components of the dangling bond state.

The photoemission intensities are calculated with the golden rule formula of the one-step formulation of photoemission. The final state is a time-reversed LEED state. To compute it, the solutions of the complex band structure inside the crystal are matched to the correct asymptotic behaviour in the vacuum.

The measurements are carried out with unpolarized HeI$_\alpha$-radiation ($h\nu =$ 21.22 eV) using an energy analyser mounted on a two-axis-goniometer. The sample is kept fixed during the computer controlled rotation of the electron analyser. The energy resolution of the analyser is chosen to be 130 meV, which allows fast measurements. The angular acceptance is about $\pm 0.5°$ and the accuracy of the angular adjustment was $\pm 0.1°$. The sample is a UHV-cleaved GaAs single crystal.

The study of the azimuthal dependence of the photocurrent becomes less instructive for scans through high symmetry points at energies corresponding to the band extrema. There the high SDOS would dominate the spectrum. Therefore, we choose a circle in the Brillouin zone slightly off the high symmetry points, with an emission angle of 17.3° and a binding energy of -0.75 eV.

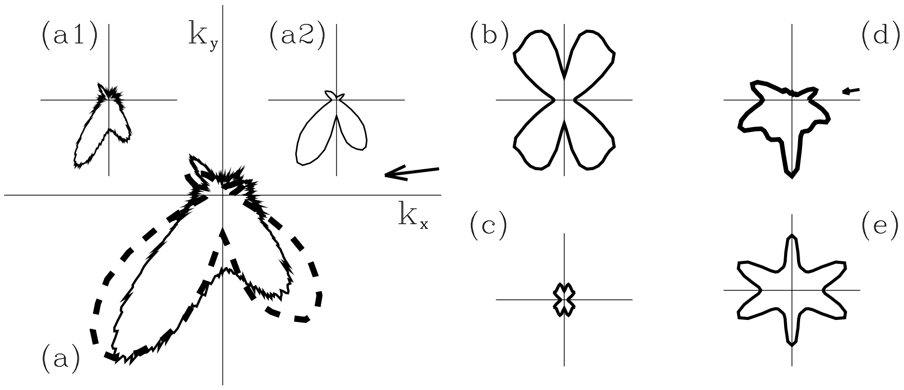

Figure 2: Photocurrent and SDOS of the dangling bond band: (a) measured (solid, a1) and calculated (dashed, a2) current for binding energies of -0.9 eV (experiment) and -0.75 eV (theory) and an azimuthal incidence of light of 8°; (b) SDOS of the uppermost layer (As) at -0.75 eV; (c) SDOS of the second layer (Ga) at -0.75 eV; (d) calculated current at -0.9 eV; (e) SDOS of the first layer at -0.9 eV. k_x and k_y indicate the orientation. In the polar plots, the radius represents the intensity of the current or the value of the SDOS. The angle is the azimuthal angle of the emission or of the k-vector. The calculations were performed with an inverse lifetime of 0.1 eV. Finally, the intensities and densities were convoluted with a Gaussian resolution of 0.03 eV.

The resulting path and the contour level of this energy are plotted in Fig. 1a. The crossings with the band and the path through areas of higher SDOS near the band result in the SDOS shown in the polar plots of Fig. 2b and 2c. All contributions to the dominating SDOS of the first layer, the partial SDOS of the p_y- and the p_z-orbitals, as well as that of the less important s-band, have this fourfold structure.

The theoretical and experimental photocurrents of the polar plot in Fig. 2a reproduce this structure of the peak directions. The shown currents differ in the corresponding binding energies by 0.15 eV. Compared to the achieved agreement between experiment and actual calculations [3], this remaining difference is relatively small and must be seen as a success of the presented comparison. The main reason for this difference is due to a slight inaccuracy in the calculated surface band structure, perhaps just caused by the spin-orbit coupling, which is neglected here. Since the best surface band structures of GaAs(110) still differ by up to 0.8 eV, the 0.15 eV lie in the usual range of theoretical uncertainty. Additional sources for the difference may be attributed to the calculated final state or to the experimental photoemission threshold. However, we find the effect of this energy shift to be quite astonishing. The calculated current for the binding energy of -0.9 eV in Fig. 2d differs strongly from the

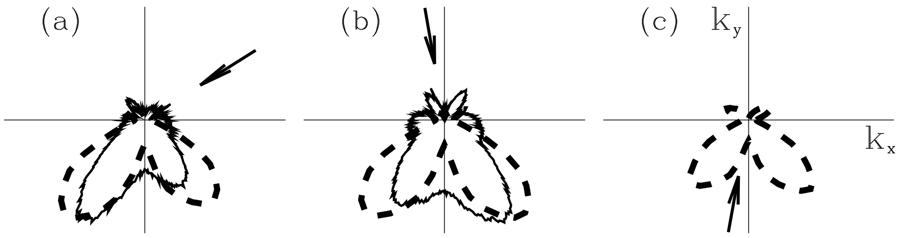

Figure 3: Photoemission intensities as in Fig. 2a for different azimuthal directions of the incident light: (a) 38°, (b) 98°, and (c) 262° (without measurement).

current for -0.75 eV of Fig. 2a.

Again, as in the case of Fig. 2a and Fig. 2b, the current for -0.9 eV in Fig. 2d reproduces the structure of the associated SDOS as plotted in Fig. 2e. The crucial dependence of the current and the SDOS on the energy dispersion allows to discriminate between the involved states and leads to the possibility of accurately tuning the theoretical bands to the experimental data.

The asymmetry between the intensities in positive and negative y-direction seems to correspond to the direction of the dangling bond, which points along the negative y-direction into the vacuum. A similar dependence is observed in angle resolved energy distribution curves of GaSb(110)[4].

The direction of the incident light causes a modulation of the intensities. The comparison of the polar plots in Fig. 3 and Fig. 2a indicates an amplification in the forward direction of the parallel part of the incoming light. This may be understood by simply regarding the value of the scalar product between the vector potential of the light and the wave vector of the outgoing electron. This scalar product is the resulting influence of the light if one assumes a constant vector potential and one plane wave as final state.

To conclude, we reported the first measurement and calculation of azimuthal valence band photoemission scans of the clean GaAs(110) surface. The azimuthal scans show distinct topologies, which seem to reflect the anisotropy of the electronic structure of the initial states. This is discussed in detail for the example of the dangling bond band. The azimuthal pattern varies strongly with binding energy.

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