Zeitschrift: Helvetica Physica Acta
Band: 62 (1989)
Heft: 6-7

Artikel: Ab-initio calculation of the anisotropic dielectric response of GaAs(110)/Sb

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DOI: https://doi.org/10.5169/seals-116118

AB-INITIO CALCULATION OF THE ANISOTROPIC DIELECTRIC RESPONSE OF GaAs(110)/Sb

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Abstract: The ab-initio pseudopotential method has been used to calculate electronic structure, dielectric tensor and surface reflectivity of a Sb monolayer deposited on GaAs(110). Due to the geometric configuration of the system the dielectric response and optical properties turn out to be strongly dependent on the polarization of the exciting field.

Surface sensitivity in optical measurements can be achieved by focusing on optical anisotropies: the simmetry breaking associated to the crystal truncation in fact makes the dielectric response strongly dependent on the polarization of the incident light. This paper presents the results of a theoretical study of the anisotropy in the surface optical spectra of the system obtained by depositing one monolayer of Sb on the cleavage surface of GaAs. This interface has been considered a model system for the theoretical and experimental study of the Scottky barrier formation since the geometry of the atoms at the interface are well characterized, presenting an ordered (1X1) structure with Sb atoms arranged along zig-zag chains resembling the geometry of Ga and As atoms at the topmost layer of the GaAs(110) surface (1)

The surface contribution to reflectivity is defined as the correction to Fresnel formula due to the real crystal truncation; as described in ref. 2 its evaluation in the single particle approximation amounts to compute i) the bulk and surface energy spectrum and ii) the transition probabilities between states of the perfect and of the truncated crystal, defining the bulk and surface dielectric tensor respectively. The present surface calculation

has been performed in the repeated slab geometry, with a slab size corresponding to 9 (110) GaAs layers plus 1 Sb layer on each side; the slabs are separated by 5 missing layers. The electronic states are determined in the local density approximation with the X_α expression of the exchange-correlation potential. Figure 1 shows the calculated density of states of GaAs(110)/Sb: states associated to Sb appears between -10 and -7 eV below the valence band maximum and around the band edges (3). A detailed comparison between theoretical band dispersion and angle resolved photoemission data (4) will be the subject of a forthcoming paper. Figure 2 shows the calculated surface reflectivity for the two polarizations of incident light, parallel and perpendicular to Sb atomic chains. The two curves present two anisotropic peacks around 2.5 and 3 eV corresponding to transitions between states localized at Sb atoms; these results are in good agreement with recent elissometry measurements (5).

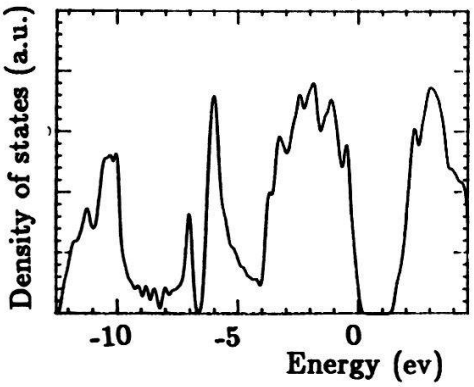

Fig.1 Density of states of one Sb monolayer deposited at GaAs(110)

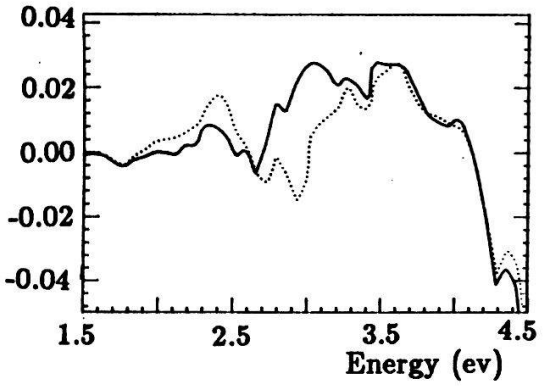

Fig.2 Surface reflectivity of GaAs(110)/Sb for light polarization along the chains (dotted line) and perpendicular to them.

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