THE DEFECT STRUCTURE OF InSb (110) SURFACES

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The defect structure, i.e. chemical, structural, and electrical properties, of InSb (110) surfaces are investigated by combined AES, RHEED, and surface conductivity studies. The surface condition determines the extrinsic states. It is found that the states are donortype and their energy is in the vicinity of the conduction band minimum.

I. Introduction

Experimental and theoretical investigations have yielded the generally accepted conclusion that no intrinsic surface states exist in the gap on the (110) faces of GaAs and other smaller band gap III-V semiconductors. However, it is well established that structures in the density of states within the gap are due to extrinsic states strongly depending on the presence of defects.

This paper is dealing with the measurements of chemical, structural, and electrical properties of clean InSb (110) surfaces as a function of surface preparation and surface charge in order to derive within the gap region the term spectra of surface states and to enhance from our investigations considerably their understanding.

II. Experimental

The investigations at various temperatures were carried out under UHV conditions at base pressures below 10^{-8} Pa after bakeout. Clean surfaces are obtained by cleaving at room temperature with the double wedge technique or by ion bombardment annealing cycles. The properties of the p-type specimens, their mounting, and the manipulator with cooling and heating facilities have been described [1-3].

The chemical, structural, and electrical properties of the surfaces have been investigated by AES, RHEED, and field effect spectroscopy. Details of the experimental set-up have been reported [1-6].

Changes of surface charge accomplish different surface potentials by variation of temperature, application of external fields, and gas adsorption. The stoichiometry and the morphology of the surfaces influences the defect structure of the surfaces by the procedure of sample preparation and treatment as cleavage, ion bombardment annealing techniques and low energy ion bombardment.

III. Results

AES shows only the presence of In and Sb on the cleaved and on the cleaned [6] surfaces. The ratio of In/Sb atoms in the surface is al-

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tered during heating and oxygen uptake. The temperature dependence of the Auger peak heights implies that annealing temperatures of less than 350 °C result in reversible changes of surface stoichiometry and temperatures higher than 350 °C in irreversible ones. The AES data [8] show during exposure a decrease of the In and Sb and a simultaneous increase of the oxygen peak height in combination with a shift of the oxygen peak to lower energies indicating chemisorbed oxygen.



Fig. 1 Density of surface states per energy interval versus energy for (110) surfaces (--- cleaved, --- cleaved and annealed, ... cleaved, annealed, and ion bombarded, -.-- cleaved, annealed, and oxygen covered): The density of states for the bulk is drawn for comparison

The RHEED patterns of the cleaved and of the cleaned surfaces generally exhibit streaks [3,5] or spots [5], which are compatible with the bulk lattice structure. The relative intensity, defined as the ratio of reflex intensity to the intensity between the reflexes, decreases gradually during heating [1,5] and oxygen exposure [7] yielding finally a diffuse background intensity.

The surface charge and the surface condition govern the location of the minimum of the electric field induced changes $\Delta\sigma_s$ of surface conductivity σ_s . Cleaved surfaces exhibit a minimum of the field induced $\Delta\sigma_s$ at positive voltages at the field plate [3]. For bad cleaves the minimum is located at lower positive voltages. Annealing

in UHV to temperatures below 350 ^OC shifts the minimum independently of the cleavage state to higher positive voltages [3]. Oxygen exposure shifts the minimum to negative voltages with simultaneous broadening of its shape [7]. Surfaces cleaned by ion bombardment annealing techniques show a minimum at negative voltages [8].

The surface states (Fig. (1)) show independently of surface preparation and of surface treatment throughout the energy gap a continuous distribution with a minimum near the middle of the gap and steep increases towards the valence band maximum (VBM) and the conduction band minimum (CBM). Depending on the surface condition more or less pronounced fine structures are superposed to the continuous distribution (Fig. (1)). A peaking distribution near CBM characterizes bad cleaves. Irrespectively of the cleavage state this structures vanishes during annealing in UHV without changing the continuous distribution [3]. Oxygen sorption changes the spectrum of surface states throughout the energy gap especially near the band edges. The surface state density near CBM increases with oxygen dose indicating a shift to higher energies [7]. The ion bombarded and annealed surfaces show in the upper half of the gap a peaking structure of surface states with high density [8].

IV. Discussion

The relation of field induced charge and surface conductivity allows the analysis of the experimental results by comparison [9] with calculations [3,5] yielding the band bending at the surface. Cleaved surfaces exhibit a downward band bending depending on the cleavage state. Heating of cleaved surfaces results in an upward band bending saturating irrespectively of the cleaving state at the same value of the surface potential near flat bands. Oxygen uptake and ion bombardment pronounce the downward band bending yielding finally electron conduction in the space charge layer.

The results are understood on the base of intrinsic and extrinsic surface states [9]. The U-shaped density of states has intrinsic character because all the surfaces show this distribution. The peaking structures are of extrinsic character because the density and the energy of these states depend on the surface conditon.

The analyses of LEED intensities have revealed that the clean InSb (110) surface exhibits a structural rearrangement [10]. The rearrangement of surface atoms follows electronic rearrangements leading to the generally accepted model [11] of surface state bands: empty In derived surface states in the conduction band region and filled Sb derived surface states in the valence band region. The surface states, splitt off from the non-localized states in the bulk bands, degenerate by changes of boundary conditions [12] into a continuous distribution of intrinsic localized states in the gap [3,9].

AES and RHEED give no indication either for elements other the constituents of the compound semiconductor or for excess In or Sb. Thus, the extrinsic states of cleaved and cleaned surfaces originate from defects or from impurities. The correlation between the Auger peak height, the weakening of the RHEED diffraction spots, and the electronic properties imply that the extrinsic states of oxygen covered surfaces are related to the adsorbate.

The U-shaped distribution of intrinsic states has shown that the larger the spread of the boundary conditions [12] the more the surface state is located in the middle of the gap, i.e. these are the

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states with the largest disturbance of their surrounding. Small fluctuations result in states near CBM or VBM. The nature of the source responsible of the gap state determines the energy of the states. The concentration of the sources governs their density. The disorder in the surface may be caused by point defects like empty sites or single atoms on top of the surface, line defects like atomic steps or domain boundaries of superstructure, and complex defects like clus-ters or microcracks. The impurities may be adsorbed from the residual gas atmosphere or diffuse out of the bulk. The gases are intentionally adsorbed on the surfaces. Defects, impurities, and adsorbates pro-duce distortions in the surface. The new arrangement of surface atoms introduces by strains a second reordering of electrons between the surface atoms originating in extrinsic surface states.

The results (Sec. (3)) yield two main features for the extrinsic states: (i) the energy is around CBM within the upper half of the gap or the conduction band region, (ii) the charging character is donortype. The extrinsic surface states probably change the electronic structure within the valence band region which cannot be detected because of experimental limitations.

In addition to the experimental conditions for the occurence of the extrinsic states calculations of other authors [13] give some evidence for the identification of the states. The calculations have investigated the gap states on (110) faces associated with defects having one and two dangling bonds on either metallic or non-metallic atoms. Extrapolating the theoretical results from InP and InAs to InSb the states within the conduction band region correspond to In atoms with one and two dangling bonds.

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