Surface electronic structure of InAs(110)

C. B. M. Andersson

Materials Science, Royal Institute of Technology, S-100 44 Stockholm, Sweden

J. N. Andersen

Department of Synchrotron Radiation Research, Institute of Physics, Lund University, Sölvegatan 14, S-223 62 Lund, Sweden

P. E. S. Persson

National Supercomputer Center, University of Linköping, S-581 83 Linköping, Sweden

U. O. Karlsson

Materials Science, Royal Institute of Technology, S-100 44 Stockholm, Sweden

The electronic structure of the InAs(110) cleavage surface has been studied by angle-resolved photoelectron spectroscopy. The bulk band structure has been calculated utilizing the augmented plane-wave method and then the bulk bands have been projected along the lines $\bar{\Gamma}$-$\bar{X}$ and $\bar{\Gamma}$-$\bar{Y}$ of the surface Brillouin zone (SBZ). Three surface-related structures have been found and their initial state versus $k_\parallel$ dispersion along the line $\bar{\Gamma}$-$\bar{X}$ and the line $\bar{\Gamma}$-$\bar{Y}$ of the SBZ has been determined. The structures are identified as A_5, A_4, and A_3 along $\bar{\Gamma}$-$\bar{X}$ and as A_5, A_4, and C_2 along $\bar{\Gamma}$-$\bar{Y}$.

Although the zinc-blende (110) surfaces show simple 1×1 low-energy electron-diffraction (LEED) patterns, their geometrical structure is known to be far from ideal.[1-3] Instead, the surface is characterized by a movement of the anions out of the surface plane and the cations into the crystal introducing a bond rotation angle of $27° \leq \omega_1 \leq 31°$. These structural rearrangements of the surface atoms also have a substantial influence on the surface electronic structure. The anion-derived dangling-bond state is pushed down to or below the valence-band maximum, and new surface-related electron states are created. Several calculations of the surface electronic structure of the zinc-blende (110) surfaces have been performed but the agreement with experimental data is still not satisfactory. One reason for this is that the interpretation of the photoemission spectra is difficult due to the fact that the contributions from surface-related structures are often hidden by emission from strong bulk-related structures. We have investigated the surface electronic structure of the valence band of the InAs (110) cleavage surface along the $\bar{\Gamma}$-$\bar{X}$ and $\bar{\Gamma}$-$\bar{Y}$ lines of the surface Brillouin zone (SBZ) by means of angle-resolved ultraviolet photoemission spectroscopy (ARUPS). Several surface electron bands have been detected and their initial-state energy versus wave vector parallel to the surface $E_i(k_\parallel)$ dispersions have been established. To identify a surface-related structure, we have used the following criteria. It should show symmetry around the symmetry points of the SBZ and be stable in the initial-state energy when the photon energy is varied.

The ARUPS experiments were performed in a VG ADES 400 spectrometer with polarized synchrotron radiation from the DORIS II storage ring at the Hamburger Synchrotronstrahlungs labor (HASYLAB).[4] The samples were undoped [carrier concentration $(2.5-2.7) \times 10^{16}$ cm^{-3}], n-type InAs single-crystal rods, $5 \times 5 \times 20$ mm,

that were cleaved inside the vacuum chamber in ultrahigh vacuum. The quality of the sample surface was checked by LEED. Clear (1×1) patterns with sharp spots and low background were observed. LEED was also used to adjust the azimuthal angle ϕ of the sample. To get a common energy reference level, the Fermi level of Au evaporated onto the sample holder was measured for all photon energies used.

To describe the geometry of the experiment, we have adopted the labeling of angles from Huijser, van Laar, and van Rooy.[5] The mirror plane of the crystal is defined by the $\langle 001 \rangle$ and the $\langle 110 \rangle$ directions. The azimuthal angle ϕ of the sample is defined here as the angle between the $\langle 001 \rangle$ direction and the horizontal plane. When the detection angle of the outgoing photoelectrons is $\theta_e > 0°$, the detector is located on the opposite side of the surface normal compared to the incoming photons. This gives that if $\phi=0°$ and $\theta_e > 0°$, the component parallel to the (110) surface of the wave vector k of an outgoing electron $k_\parallel$, is located along the $\langle 001 \rangle$ direction. The magnitude of $k_\parallel$ is given by $k_\parallel = 0.5123 * \sin(\theta_e) * \sqrt{(E_{\text{kin}})}$ in units of Å^{-1}, where E_{kin} is the kinetic energy of the outgoing electron.

To facilitate the identification of the surface-related structures in the spectra, the electron band structure of InAs was calculated by a combination of the linear augmented plane-wave method[6] and the relativistic augmented plane-wave method.[7] The calculation was done within the density-functional theory, using the Hedin-Lundquist local-density approximation for the exchange and correlation potential.[8]

In order to establish the position of the valence-band maximum (VBM) relative to E_F, normal emission spectra were recorded over a wide photon energy range and the binding energy of the observed structures was plotted as a

function of photon energy. A comparison with the calculated bulk band structure showed that emission into primary cones dominates the spectra, as demonstrated by Williams et al.,[9] and that the difference between the Fermi level and the valence-band edge is $E_F - E_v = 0.7$ eV, i.e., the Fermi level at the surface is located in the conduction band. According to van Laar, Huijser, and van Rooy,[10] this pinning of the Fermi level in the conduction band is due to partially filled cation-derived dangling-bond states located at steps at the surface.

A selection of spectra with photon energy $\hbar\omega = 15$ eV recorded along the direction $\bar{\Gamma}$-$\bar{X}$ is presented in Fig. 1. In these spectra, several structures can be observed. We
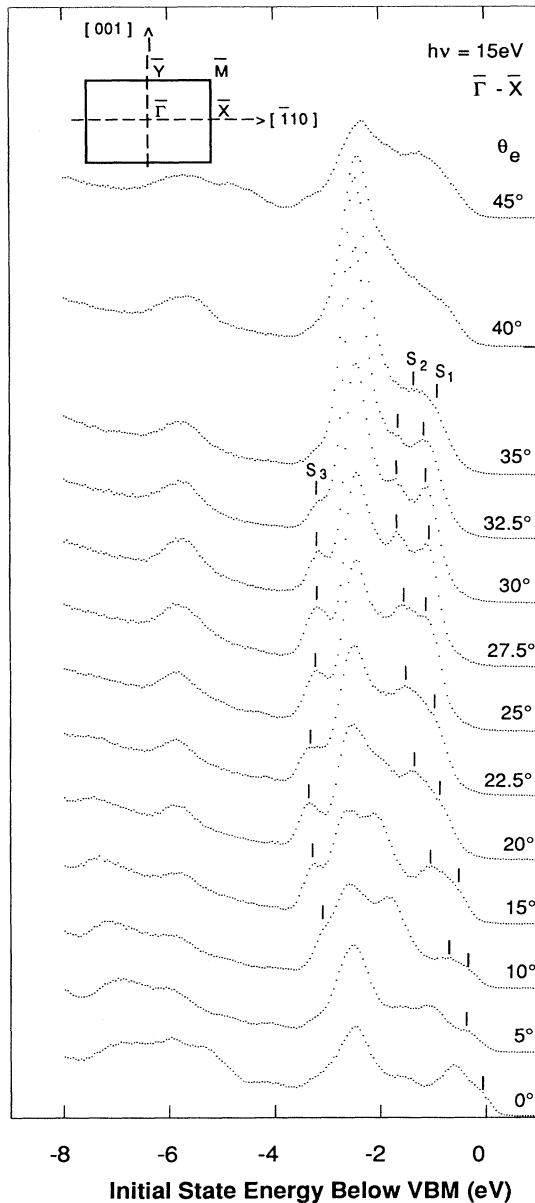

FIG. 1. Part of the angular series in the direction $\bar{\Gamma}$-$\bar{X}$ with photon energy $\hbar\omega = 15$ eV.

will only discuss surface-related structures here. For spectra with emission angle θ_e between 25° and 35°, states with an initial-state energy E_i around 1 eV below the VBM correspond to the region of the SBZ close to the $\bar{X}$ point. The topmost structure labeled S_1 located around -1.0 eV in these spectra is here clearly resolved from the next structure labeled S_2 located around -1.6 eV. Both structures disperse towards the VBM when we approach the $\bar{\Gamma}$ point, i.e., when we go from $\theta_e = 30°$ towards 0°. To determine the exact energy positions of these states in the region of $\bar{\Gamma}$ is not possible due to lifetime broadening of the surface structures and to strong bulk contributions overlapping the surface structures. The small peak S_3 shows a weak $E_i(k_\parallel)$ dispersion. It varies between -3.1 and -3.35 eV with the minimum for $\theta_e = 20°$ and 52.5° (not shown). For θ_e close to 0°, S_3 overlaps with direct transitions between bulk bands which makes it difficult to establish the $E_i(k_\parallel)$ dispersion.

Some selected spectra recorded with θ_e along the line $\bar{\Gamma}$-$\bar{Y}$ of the SBZ are presented in Fig. 2. To demonstrate the polarization dependence of the structure S_1 we show in the lower part of Fig. 2 a comparison between two spectra, both recorded with $\hbar\omega = 15$ eV. The upper spectrum was recorded with the polarization vector **A** of the incoming photons perpendicular to the $\bar{\Gamma}$-$\bar{Y}$ direction and the lower spectrum was recorded with **A** parallel to the $\bar{\Gamma}$-$\bar{Y}$ direction. The azimuthal angles ϕ of the sample and the emission angles θ_e are in both cases chosen so that $k_\parallel$ of the detected outgoing electrons are parallel to the direction $\langle 00\bar{1} \rangle$, i.e., parallel to the As dangling bond. In the spectrum with **A** parallel to the $\bar{\Gamma}$-$\bar{Y}$ direction, we have identified two surface-related structures, labeled S_1 and S_2 in the figure. The energy positions of the structures S_1 and S_2 are in these spectra, -0.80 and -1.10 eV, respectively. In the spectrum with **A** perpendicular to the $\bar{\Gamma}$-$\bar{Y}$ direction, the peak S_1 has vanished. The uppermost contribution to this spectrum is for this polarization case the state S_2.

The upper part of Fig. 2 shows a comparison between spectra recorded along $\bar{\Gamma}$-$\bar{Y}$ with the azimuthal angle of the sample $\phi = 0°$ or 180°. For all these spectra, the photon energy is $\hbar\omega = 17$ eV and the polarization vector **A** is parallel to the line $\bar{\Gamma}$-$\bar{Y}$. It is clearly seen that some structures in these spectra are sensitive to the choice of the azimuth. They show the same azimuthal dependence as the GaAs spectra published by Huijser, van Laar, and van Rooy.[5] The structure S_1 is pronounced for two combinations of θ_e and ϕ, i.e., for $\theta_e > 0°$ and $\phi = 180°$ or $\theta_e < 0°$ and $\phi = 0°$. For other combinations of azimuthal angles and emission angles, S_1 appears as a very weak shoulder or is nondetectable. For θ_e around 0°, the peak S_4 is pronounced in these spectra only for $\phi = 0°$. For $\theta_e = 19°$ and $\phi = 0°$, it shows as a very weak structure.

The experimentally obtained $E_i(k_\parallel)$ dispersion along the line $\bar{\Gamma}$-$\bar{X}$ is presented in Fig. 3. The $\bar{X}$ point, which is a symmetry point of the SBZ, is marked with a solid line. The other solid lines indicate the projection of the calculated bulk bands. The uppermost line shows the projection of the top of the topmost bulk energy band. The symmetric area inside the solid lines is the open lens

where no bulk-related electron states should be found. All states are symmetric around the $\bar{X}$ point and the $E_i(k_\parallel)$ dispersions for these structures are the same for all four photon energy series recorded. Thus we conclude that these states are surface related. The structure S_1 located around -1.0 eV at the $\bar{X}$ point is clearly identified
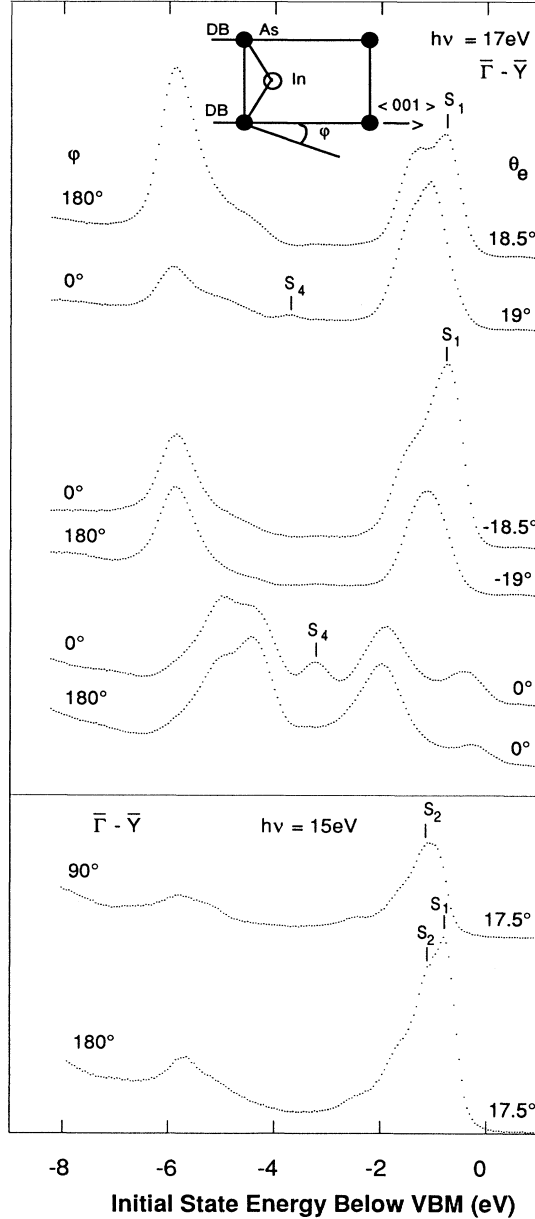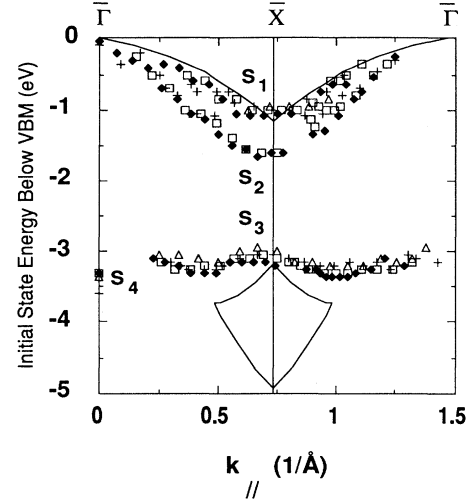

FIG. 3. Initial-state energy E_i relative to the valence-band maximum as a function of $k_\parallel$ for the experimentally obtained surface electronic structure along the line $\bar{\Gamma}$-$\bar{X}$. The data points are labeled as follows: ♦, 15 eV; □, 17 eV; +, 20 eV; and △, 23 eV.

as a surface state at the $\bar{X}$ point because it disperses into the bulk band gap at $\bar{X}$, according to our bulk band calculation. For other parts of the line $\bar{\Gamma}$-$\bar{X}$, it is a surface resonance. The next structure S_2 located around -1.6 eV at the $\bar{X}$ point, is a surface resonance everywhere. Both S_1 and S_2 disperse upwards towards $\bar{\Gamma}$. It is hard to determine the energy position of these states with accuracy for other parts of the SBZ than the region around the $\bar{X}$ point, because the states are not clearly resolved in
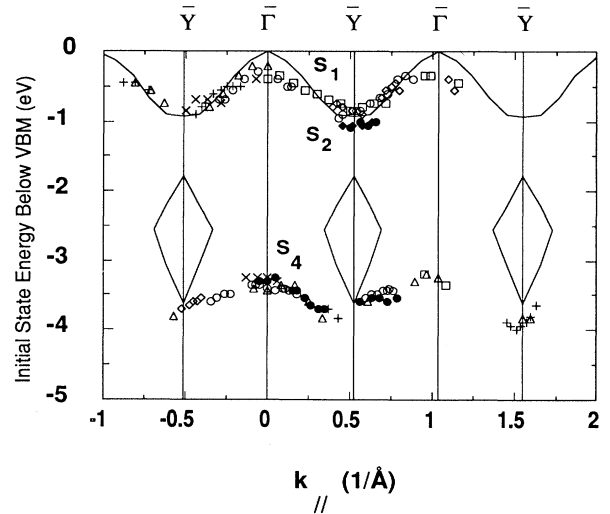

FIG. 2. Comparison between spectra recorded for different polarization cases and detection geometries. The lower part of the figure shows spectra recorded for $\hbar\omega=15$ eV along the $\bar{\Gamma}$-$\bar{Y}$ direction. The upper spectrum was recorded with the polarization vector **A** perpendicular to the $\bar{\Gamma}$-$\bar{Y}$ direction and the lower spectrum was recorded with **A** parallel to the $\bar{\Gamma}$-$\bar{Y}$ direction and $\phi=180°$. The upper part shows a comparison between spectra recorded along $\bar{\Gamma}$-$\bar{Y}$ with the rotation angle of the sample $\phi=0°$ or 180°. The comparison is made for three different detection geometries $\theta_e<0$, $\theta_e>0$, and $\theta_e=0$.

FIG. 4. Initial-state energy E_i relative to the valence-band maximum as a function of $k_\parallel$ for the experimentally obtained surface electronic structure along the line $\bar{\Gamma}$-$\bar{Y}$. Data points with **A** perpendicular to the mirror plane are labeled as follows: ●, 13 eV; ♦, 15 eV. Data points with **A** parallel to the mirror plane and $\phi=180°$ are labeled as follows: ○, 13 eV; ◇, 15 eV; and □, 17 eV. Data points with $\phi=0°$ are labeled as follows: ✕, 17 eV; +, 20 eV; △, 23 eV; and ▲, 26 eV.

other parts of the SBZ, as can be seen in Fig. 1. The structure S_3 located around -3.1 eV around the $\bar{X}$ point is a surface resonance in the entire SBZ. The initial-state energy goes through a local minimum at -3.35 eV halfway between $\bar{\Gamma}$ and $\bar{X}$. When we approach $\bar{\Gamma}$, the dispersion is hard to establish as can be seen in Fig. 1. The structure S_4 is located around -3.35 eV at $\bar{\Gamma}$. We have not been able to establish its dispersion along $\bar{\Gamma}$-$\bar{X}$.

The experimentally obtained $E_i(k_\parallel)$ dispersion along the line $\bar{\Gamma}$-$\bar{Y}$ is presented in Fig. 4. We have identified three surface-related structures. The structure S_1 has its maximum at the $\bar{\Gamma}$ point at -0.3 eV. It disperses down towards the $\bar{Y}$ point where it is found at -0.85 eV. This state is sensitive to the direction of the polarization and the experimental geometry as described above. The energy position of S_2 close to the $\bar{Y}$ point is estimated to -1.05 eV, i.e., 0.2 eV below S_1. The energy position of S_2 is hard to determine for other parts of the $\bar{\Gamma}$-$\bar{Y}$ line than the $\bar{Y}$ point because when $\mathbf{A}$ is parallel to the mirror plane the emission from S_1 is dominating, and when $\mathbf{A}$ is perpendicular to the mirror plane the emission from the highest-lying bulk energy band, which has odd symmetry, is strong and overlaps with the back bond state.[11,12] The structure S_4, located around -3.35 eV at $\bar{\Gamma}$ and around -3.7 eV at $\bar{Y}$, is seen in spectra with a photon energy of 13 eV for all detection angles. In Fig. 2 it is seen in the spectrum with $\hbar\omega = 17$ eV, $\phi = 0°$, and $\theta_e = 0°$. For other photon energies, it is detected for $\phi = 180°$ negative detection angles, or $\phi = 0°$ positive detection angles.

From a comparison with theoretically calculated surface state bands,[2,3] we conclude that our experimental data for S_1 and S_2 correspond very well to the calculated dispersions of the dangling-bond state denoted as A_5 and the back bond state denoted as A_4. In this notation system, A_i denotes states mainly associated with the anions and C_i denotes states mainly associated with the cations. For InAs, the anion is As and the cation is In.

The polarization dependence of the state S_1, shown in the lower part of Fig. 2, is in agreement with the expected behavior of the dangling-bond state A_5. For the ideal (110) surface, the dangling-bond state located on the anion is filled and has components along the $\langle 00\bar{1}\rangle$ and

the $\langle 110\rangle$ directions, while the dangling-bond state on the cation is empty. In the spectrum with $\mathbf{A}$ perpendicular to the $\bar{\Gamma}$-$\bar{Y}$ direction, the state S_1 is not excited. This polarization dependence is expected because the cross section for the excitation of an electron goes down when the $\mathbf{A}$ vector is perpendicular to the direction in which the state is extended. The identification of the structure S_3 is not as clear as for the states S_1 and S_2, because we are not able to follow the state through the entire SBZ and the theoretically calculated surface states do not coincide with our experimental data points. We tentatively attribute this structure to the state A_3 which is the one that comes closest. The calculations presented in Refs. 2 and 3 also indicate that the structure S_3 goes through the open lens of the bulk band structure in the area around the $\bar{X}$ point and thus should be a surface state in this region, and a surface resonance elsewhere. This is contradictory to the calculation made by us which indicates that this state is situated immediately above the open lens and thus is a surface resonance in the entire SBZ. The identification of the structure S_4 is also unreliable; it is tentatively identified as C_2. We have not managed to follow this structure along the line $\bar{\Gamma}$-$\bar{X}$. According to the surface band-structure calculations, the state C_2 disperses rapidly downwards from $\bar{\Gamma}$ to $\bar{X}$ into an energy region where it is hard to separate from the bulk band contribution.

In conclusion, we have identified four surface-related structures in the ARUPS spectra of the InAs(110) surface. All states, except the dangling-bond state, are surface resonances according to our bulk band-structure calculation. The dangling-bond state is a surface state in the regions close to $\bar{X}$ and $\bar{Y}$ while it is a surface resonance close to $\bar{\Gamma}$. The spectra are mainly dominated by primary cone emission from the bulk and contributions from regions with a high density of states.

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