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## Occupied surface-state bands of the $(1 \times 2)$ ordered phase of Bi/InAs(110)

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**Abstract.** The ordered  $(1 \times 2)$  monolayer of Bi on the InAs(110) surface is studied by means of angle-resolved high-resolution ultra-violet photoemission at room temperature. Four bands of Bi-induced surface states are singled out and their dispersion is mapped along the high-symmetry directions of the surface Brillouin zone. The highest occupied state  $S^I$  lies inside the InAs(110) energy gap at 0.2 eV binding energy and spreads across the Fermi level, determining the semimetallic character of the system. The second-highest occupied state  $S^{II}$  is located at 0.83 eV binding energy (at  $\bar{\Gamma}$ ), while states  $S^{III}$  and  $S^{IV}$  are located near the internal gap edge at 2.57 eV and 3.3 eV binding energy, and present band dispersions along  $\bar{\Gamma}\bar{X}$  of  $\sim 340$  meV and 300 meV, respectively. The Bi-induced bands of the  $(1 \times 2)$  phase are shifted in energy relative to the corresponding bands of the  $(1 \times 1)$ -Bi/InAs(110) phase and their width is reduced. These differences are discussed in the light of the geometric structure of the two phases.

The  $(1 \times 1)$  phases of group V semimetals grown on III–V(110) surfaces have been widely addressed in the past as a model system for studying the electronic properties of *ideal* metal/semiconductor interfaces [1]. Group V semimetals in fact grow unreactively on semiconductor surfaces, forming ordered and stable monolayers at room temperature (RT). Great efforts have been made to characterize these systems, both from an experimental and from a theoretical point of view. All the  $(1 \times 1)$ -V/III–V(110) systems have similar geometric structures, which can be described within the so-called epitaxial continued-layer structural (ECLS) model [2]. In this model the clean-surface relaxation is lifted and the adatoms continue the underlying substrate bulk-like structure forming zigzag chains along the  $[1\bar{1}0]$  direction. These systems show a semiconducting character, with adatom-related electronic states partially spreading inside the fundamental energy gap.

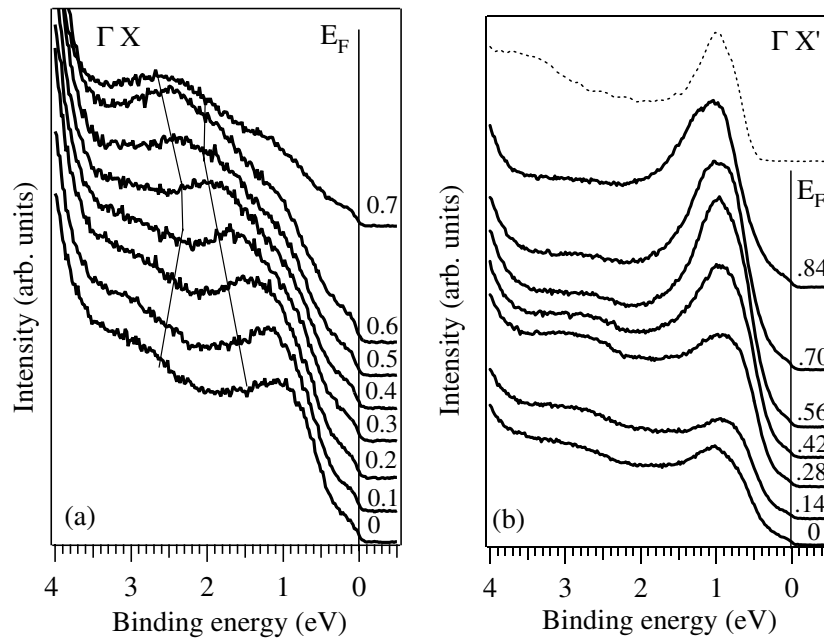
Recently, it has been recognized that Bi/III–V(110) systems can display other ordered and stable phases, characterized by surface reconstruction. In particular, some attention has been paid to the  $(1 \times 2)$ -Bi/GaSb(110) and  $(1 \times 2)$ -Bi/InAs(110) surfaces, obtained as stable phases after an appropriate annealing procedure. Their geometrical structures have been investigated [3, 4], and it has been shown that in both systems a substrate missing-row reconstruction occurs, in which one substrate row in every two along the  $[001]$  direction is missing and the Bi zigzag chains are strongly tilted towards the groove left in the restructured substrate. Angle-integrated photoemission measurements have shown that both interfaces,

unlike the  $(1 \times 1)$  phases, display a semimetallic character, with Bi-induced electronic states at the Fermi level [5, 6].

In this article we report an angle-resolved photoemission study of the  $(1 \times 2)$ -Bi/InAs(110) system. The Bi-induced-state dispersion is mapped along the high-symmetry directions of the surface Brillouin zone (SBZ) and compared with that of the  $(1 \times 1)$ -Bi/InAs(110) phase. This comparison among 2D-ordered systems which only differ in their geometrical structure gives some insight into the mutual influence of their structural and electronic properties.

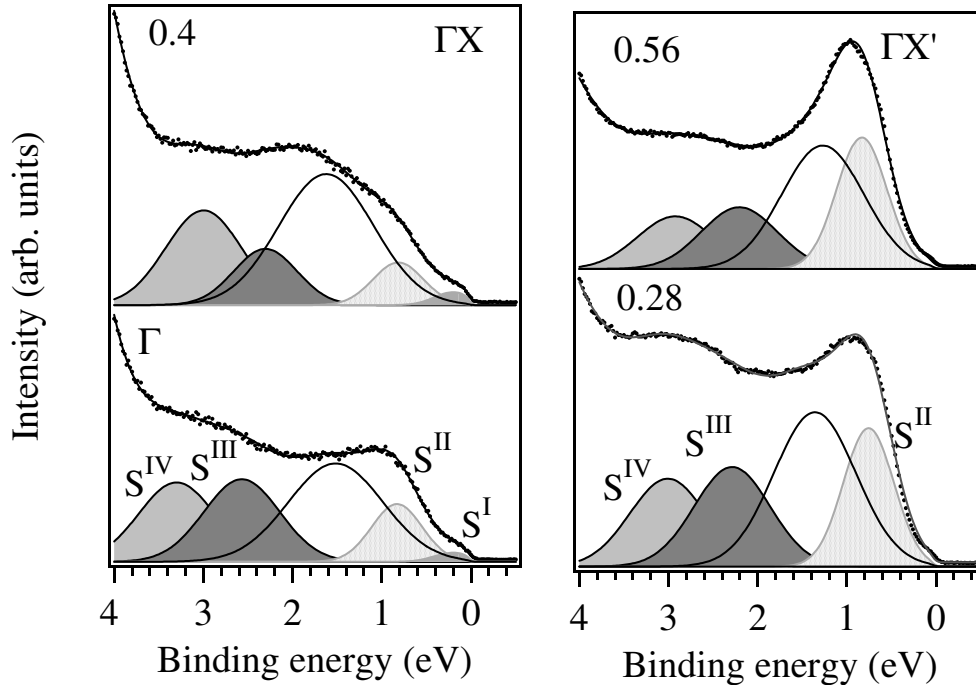
Measurements were performed at Lausanne in a UHV environment (base pressure:  $2 \times 10^{-10}$  mbar) using a He discharge source, with photon energy of 21.218 eV (He I $\alpha$ ). Angle-resolved valence band photoemission measurements were performed, rotating the crystal along the azimuthal axes with an angular resolution of  $1^\circ$ . The photoemitted electrons were analysed with a hemispherical analyser (SCIENTA SES-300) with an instrumental energy resolution of 15 meV at 10 eV pass energy. The position of the Fermi edge was evaluated to better than 2 meV by measuring the spectrum of an evaporated Ag polycrystalline film. The n-type doped InAs(110) single crystal ( $n \sim 10^{18}$  cm $^{-3}$ ) was cleaved in air and clean InAs(110) surfaces were prepared by cycles of Ar $^+$  sputtering and slow annealing to 400 °C, while the absence of contaminants was checked by x-ray photoemission measurements. Bi was evaporated on the substrate at RT from a resistively heated quartz crucible, previously calibrated. The  $(1 \times 2)$  phase was obtained from a thick (20 ML) Bi film, previously deposited at RT, slowly annealed to 250 °C in order to allow the Bi rearrangement and partial desorption. This procedure has been shown to lead to a well-ordered  $(1 \times 2)$  structure in a fully reproducible way, as has been checked by LEED and GIXD measurements [4, 5].

Angle-resolved photoemission measurements of the  $(1 \times 2)$ -Bi/InAs(110) phase along the  $[1\bar{1}0]$  ( $\bar{\Gamma}\bar{X}$ ) and  $[001]$  ( $\bar{\Gamma}\bar{X}'$ ) directions are shown in figure 1. In order to identify the Bi-induced electronic states in the valence band spectra, we compare with both the clean-surface valence band (upper curve, dotted line in figure 1(b)) and to previous photoemission measurements (angle-integrated around the  $\bar{\Gamma}$  point) [5]. The clean-InAs-surface electronic states can be identified in the valence band spectrum (dotted line) as the shoulder located at 0.75 eV binding energy (BE) (state A $_{4-5}$ ) and the broad feature located around 3.5 eV, in agreement with previous literature [7, 8]. The main-feature distributions of the clean InAs surface and  $(1 \times 2)$ -Bi valence bands are rather similar. Nonetheless, we can identify three features as Bi-induced states. The lowest-binding-energy one can be clearly detected as a foot spreading inside the whole substrate fundamental gap, confirming the semimetallic character of this phase [5]. It is more intense along the  $\bar{\Gamma}\bar{X}$  direction than along  $\bar{\Gamma}\bar{X}'$ . The second one is located near the valence band edge around 0.8 eV and appears as a shoulder, similarly to the A $_{4-5}$  state of the clean surface and in agreement with reference [5]. The feature at highest binding energy appears as a broad peak located approximately around 3 eV binding energy, displaying a similarity with the clean-surface feature at 3.5 eV. This structure is actually formed by two peaks, as can be inferred from the spectra taken at 10% and 50% of the SBZ edge along  $\bar{\Gamma}\bar{X}$  (figure 1(a)), and by comparison with angle-integrated measurements [5]. Along  $\bar{\Gamma}\bar{X}$ , the broad peak around 3 eV disperses towards smaller binding energy and partially merges with a downward-dispersing and intensity-increasing bulk feature, located around 1–2 eV, as we shall see in the following analysis. In order to determine the energy positions of the Bi-induced states, following their dispersion along the high-symmetry directions, a non-linear lineshape analysis technique is performed, in which the photoemission lines are treated as Gaussian functions and the secondary-electron background is approximated by an exponential function included in the fit. A similar procedure has also been performed to study the band dispersion of the clean InAs(110) surface [7]. In figure 2, a selection of spectra along  $\bar{\Gamma}\bar{X}$  and  $\bar{\Gamma}\bar{X}'$  are shown, along with their best-fit curves. The best fits are performed introducing five Gaussian



**Figure 1.** Angle-resolved valence band photoemission spectra of the  $(1 \times 2)$ -Bi/InAs(110) phase, taken at angles corresponding to different fractions (indicated in the figure) of the SBZ edge along the  $\bar{\Gamma}\bar{X}$  (a) and  $\bar{\Gamma}\bar{X}'$  (b) directions. Spectra are shifted vertically for the sake of clarity. The vertical line corresponds to the Fermi level energy while the solid lines are guides showing the dispersion of the projected bulk feature and the lower-lying Bi-induced states. The upper curve (dotted line) in panel (b) is the clean-InAs-surface valence band, taken at the  $\Gamma$  point. The valence band edge of the clean surface is located 0.44 eV below the Fermi level.

functions, and allowing variation of their energy positions and intensities. The number of peaks used is the minimum necessary for fitting the spectra consistently. The Gaussian width of each peak is determined by the best-fit procedure and kept fixed for all spectra. The four peaks related to Bi-induced states are indicated in figure 2 as shadowed peaks and are labelled from lower to higher binding energies as  $S^I$ ,  $S^{II}$ ,  $S^{III}$  and  $S^{IV}$ . The fifth Gaussian peak around 1–2 eV, reported as a solid line in figure 2, accounts for the bulk state contribution, and is therefore quite broad (0.75 eV). The two highest occupied states have Gaussian width of 0.4 eV, while the two lower-lying states, that are resonant with the projected bulk band, are broader (0.6 eV). These values are in agreement with those determined for the clean-InAs(110)-surface states in reference [7]. The fitting procedure clearly shows that two peaks are needed to reproduce the broad peak located at around 3 eV BE. In fact, fitting with only one peak would require an unrealistically large peak width, compared with that of the other Bi-induced structures. On the other hand, due to the broadness of the feature around 3 eV, the uncertainty in the energy determination of states  $S^{III}$  and  $S^{IV}$  is larger than that of the highest occupied states  $S^I$  and  $S^{II}$ . The band dispersion thus obtained is shown in figure 3. The surface band position relative to the projected bulk band structure is fixed from the energy position of the clean-surface valence band edge relative to the Fermi level, as extrapolated from the clean-surface valence band spectra. Along the  $\bar{\Gamma}\bar{X}'$  direction the fitting procedure indicates that the small intensity in the spectra at the Fermi level is mainly determined by the tail of the  $S^{II}$  state, while the best-fit value of the  $S^I$  intensity is almost negligible. For this reason the dispersion of  $S^I$  is shown in figure 3 only along  $\bar{\Gamma}\bar{X}$ .

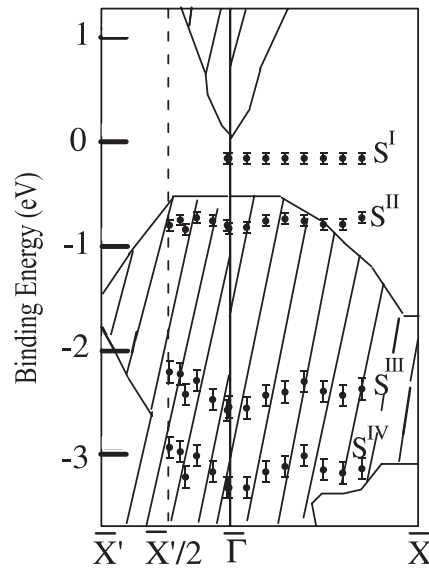


**Figure 2.** Valence band photoemission spectra (filled circles) along  $\bar{\Gamma}\bar{X}$  (left-hand panel) and  $\bar{\Gamma}\bar{X}'$  (right-hand panel), together with their best-fit curve (solid line). The Voigt components used in the fitting are also shown; shadowed peaks correspond to Bi-induced states (see the text for details). The numbers in the panels are the values of the parallel wavevector at the binding energy of  $S^{II}$ , indicated as fractions of the SBZ edge in the corresponding direction.

As far as we know, theoretical evaluation of the band structure of the  $(1 \times 2)$ -Bi phases has not been performed. In order to discuss our results we can compare to the  $(1 \times 1)$ -Bi/InAs(110) band structure calculated by Umerski and Srivastava [9]. According to them, as well as to previous works on other  $(1 \times 1)$ -V/III-V(110) phases [10], the two Bi-induced highest occupied states (labelled as  $S_7$  and  $S_8$  in reference [9]) are almost degenerate along the  $\bar{\Gamma}\bar{X}'$  direction and are located near the valence band edge. They can be related to the p orbitals located on both types of Bi atom (cation- and anion-bonded), with bonding ( $S_7$ ) and antibonding ( $S_8$ ) character. Along the  $\bar{\Gamma}\bar{X}$  direction the two states are instead well separated; in the  $\bar{X}$  region,  $S_7$  is derived from a bonding configuration between a Bi p orbital and its anion neighbour, while  $S_8$  derives mainly from a p dangling bond on the cation-bonded Bi atom. Angle-resolved photoemission measurements [11] for the  $(1 \times 1)$ -Bi/InAs(110) phase are in partial agreement with these theoretical results, showing an almost complete degeneracy between the two highest occupied states in both the SBZ high-symmetry directions. This degeneracy has also been observed in our previous measurements integrated in the region around  $\bar{\Gamma}$  [5].

States  $S_7$  and  $S_8$  of the  $(1 \times 1)$  phase can be compared to the two highest occupied states  $S^I$  and  $S^{II}$  of the  $(1 \times 2)$  phase. These latter are clearly non-degenerate, as shown in figure 3. Along  $\bar{\Gamma}\bar{X}$  the spectral density related to the highest occupied state  $S^I$  displays a maximum located at  $0.2 \pm 0.05$  eV BE and spreads across the whole InAs(110) energy gap, thus determining a finite density of states at the Fermi level $\dagger$ . The second-highest occupied state

$\dagger$  Further measurements taken at 75 K show that the system remains semimetallic also at low temperature.



**Figure 3.** The Bi-induced-state band dispersion referenced to the sample Fermi level of the  $(1 \times 2)$  phase. The symbols show the experimentally determined dispersions for  $S^I$ ,  $S^{II}$ ,  $S^{III}$  and  $S^{IV}$ . The hatched regions are the theoretical bulk band projections from reference [10] for the clean InAs(110). The dashed line indicates the SBZ folding due to reconstruction.

$S^{II}$  has a binding energy of 0.84 eV at  $\bar{\Gamma}$  (lying therefore below the InAs valence band edge), and shows a small dispersion ( $\sim 0.1$  eV) along each direction. The partial energy degeneracy between the two highest occupied states  $S_7$  and  $S_8$  in the  $(1 \times 1)$  phase is thus completely lifted in the  $(1 \times 2)$  phase, partly because each electronic state is split into two branches by the folding of the SBZ induced by the surface reconstruction. Moreover, the structural changes of the Bi chains in the  $(1 \times 2)$  phase have also to be taken into account: while in the  $(1 \times 1)$  phase each chain is in fact built by Bi atoms bonded alternately to anion and cation substrate atoms, in the  $(1 \times 2)$  phase Bi atoms in each chain are all bonded to the same kind of substrate atom [4]. This causes the  $S^I$  and  $S^{II}$  states to localize on cation-bonded and anion-bonded Bi chains, respectively, changing their character at least partially and influencing their energy splitting. This localization of the two highest occupied states on different Bi chains might also explain their different intensity behaviours as functions of the azimuthal angle (i.e. along  $\bar{\Gamma}\bar{X}$  and  $\bar{\Gamma}\bar{X}'$ ), if final-state diffraction effects are taken into account. Due to these effects, in fact, the photoelectron intensity of valence band states can be strongly dependent on the local geometric arrangement surrounding the hole left by the photoemitted electron [12].

The two lower-lying states  $S^{III}$  and  $S^{IV}$  of the  $(1 \times 2)$  phase can be compared to states  $S_6$  and  $S_5$  of the  $(1 \times 1)$  phase described in reference [9]. These are located near the internal gap edge and are nearly degenerate [9, 11]. Their character can be mainly related to the p orbitals of the first-substrate-layer As atom. The degeneracy of these states is also lifted in the reconstructed  $(1 \times 2)$  phase, probably due to the SBZ folding. Moreover, states  $S^{III}$  ( $2.57 \pm 0.05$  eV BE at  $\bar{\Gamma}$ ) and  $S^{IV}$  ( $3.3 \pm 0.1$  eV BE at  $\bar{\Gamma}$ ) are both shifted to lower binding energy relative to the corresponding  $S_6$  and  $S_5$  states in the  $(1 \times 1)$  phase. Along the  $\bar{\Gamma}\bar{X}$  direction, both  $S^{III}$  and  $S^{IV}$  bands display a sizable dispersion (0.34 and 0.3 eV of the bandwidth, respectively), though smaller than that of the corresponding  $(1 \times 1)$ -phase states. Along  $\bar{\Gamma}\bar{X}'$  this narrowing is more pronounced, probably due to the SBZ reduction in this direction.

In conclusion, the Bi-induced electronic states of the  $(1 \times 2)$ -Bi/InAs(110) system can be related to those of the  $(1 \times 1)$  phase. The structural changes introduced by the reconstruction are reflected in both an energy shift of the Bi-induced states and a reduction of their bandwidth.  $S^{\text{III}}$  and  $S^{\text{IV}}$ , which are mainly derived from the orbitals of the anion substrate atoms, decrease their binding energy in the reconstructed phase, while  $S^{\text{II}}$ , which is related to the p orbitals of the anion-bonded Bi atoms, increases its binding energy. This seems to indicate a partial charge redistribution induced by the reconstruction, with increased electron density near to the anion atoms in the first substrate layer. The surface reconstruction also causes a change in the orbital character of the highest occupied interface states, causing their energy splitting and the semimetallicity of the system. The dispersion widths of all Bi-induced states in the  $(1 \times 2)$  phase are significantly smaller than those of the  $(1 \times 1)$  phase [11]. This band narrowing could also be related to the Bi-induced-state localization on the cation- and anion-bonded chains induced by the reconstruction. Now that the geometry and the experimental dispersions of the  $(1 \times 1)$  and  $(1 \times 2)$  phases are known, theoretical calculations are required in order to elucidate the mechanism inducing the  $(1 \times 2)$  surface reconstruction and the role of the Bi-induced-state localization in determining the electronic properties of the  $(1 \times 2)$  phase.

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