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# Angle-resolved photoemission of InSb(111)–2 × 2

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**Abstract.** The electronic band structure of InSb(111) along the Γ–Λ–L⟨111⟩ direction was determined using angle-resolved photoemission spectroscopy for the photon energy between 9 and 39 eV via synchrotron radiation. The bulk band dispersion is in agreement with earlier theoretical calculations. The In- (group III-) terminated InSb(111) surface shows surface Umklapp transitions and reflection of the bulk density of states. We found two nondispersive features which were not reported before. They are related to the surface state and the resonance process of the InSb(111)–2 × 2.

Investigations of electronic properties of III–V compound semiconductors have mainly been focused on the nonpolar (110) surfaces because the clean surface is easily obtained by natural cleavage [1, 2]. On the other hand, fewer studies have been done for polar {111} surfaces in spite of their importance in electronic device applications. Two kinds of {111} surface (group III-terminated (111) and group V-terminated $(\bar{1}\bar{1}\bar{1})$ surfaces) show various reconstructions, depending upon the surface preparation conditions [3, 4]. The (111) face reveals only (2 × 2) reconstruction and its atomic geometry is proposed to be a group III-vacancy buckling structure for GaAs [5] and InSb [6] from electron diffraction and x-ray diffraction experiments. Research into the electronic structures of GaAs(111)–2 × 2 surfaces was also carried out to determine the atomic geometry [7, 8]. However, complete experimental band mapping along Γ–Λ–L⟨111⟩ direction has not been performed for InSb(111), except for in the earlier work of Hernández-Calderón and Höchst (HH) who used several resonant photon sources [9]. In this report, we present the experimental energy bands mapped from the normal-emission spectra of the InSb(111)–2 × 2 surface using synchrotron radiation with the photon energy from 9 to 39 eV. From the experimental energy bands, we have found the true bulk band transitions, Umklapp processes, and surface-related features.

The photoemission spectra were measured at the synchrotron beam line BL6A2 of UVSOR at the Institute for Molecular Science in Okazaki of Japan using a plane grating monochromator covering the photon energy range from 5 eV to 130 eV. The angle-resolved photoemission spectroscopy (ARPES) measurement was performed in an ultrahigh-vacuum (UHV) chamber equipped with a hemispherical energy analyser, low-energy electron diffraction (LEED) optics, and an Auger electron spectrometer (AES). All of the data were collected with the electron acceptance angle of 2° and overall energy resolution of 0.15–0.25 eV. The incidence angle of the light was 45° in the $[\bar{1}\bar{1}2]$ azimuthal plane. The p-type InSb(111) was degreased in organic solvents before it was introduced into the UHV

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chamber. The cleaning of the surface was performed via repeated cycles of $Ar^+$ sputtering ($E = 500$ eV) at 200 °C and final annealing to 350 °C. The surface cleanliness was checked via a distinct (2 × 2) LEED pattern and AES spectra [10].

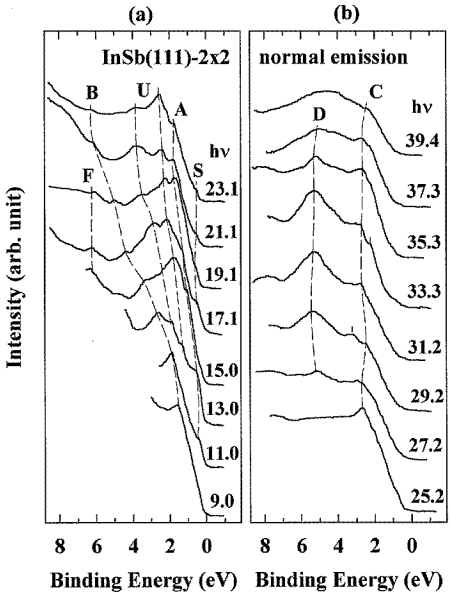


**Figure 1.** Normal-emission spectra of InSb(111)–2 × 2. (a) $\hbar\omega = 9$–23 eV; (b) $\hbar\omega = 25$–39 eV.

In figures 1(a) and 1(b) the normal-emission spectra of InSb(111)–2 × 2 are shown for photon energy $\hbar\omega$ = 9–39 eV. All binding energies are referred to the Fermi level ($E_F$) determined by the decreasing photoemission edge of thin Au film. Figure 1(a) shows several dispersive bulk-derived features for photon energy $\hbar\omega \leqslant 23$ eV. Of these features, the feature **B** rapidly disperses from $E_b = 1.5$ to 6.3 eV. The lower binding bulk features **A** are also shown for $E_b = 0.5$–1.8 eV. Other dispersive features labelled **U** each have two separable bands: one at $E_b = 1.3$–2.6 eV and the other at $E_b = 2.0$–3.9 eV. In addition, nondispersive features **F** at $E_b = 6.3$ eV and **S** at $E_b = 0.6$ eV are seen at some photon energies. At higher photon energies ($\hbar\omega > 23$ eV) in figure 1(b), we could not find any bulk band dispersion, but found two nondispersive peaks **C** at around $E_b$ = 2.8 eV and **D** at $E_b$ = 5.3 eV.

For the analysis of the experimental data, we constructed the theoretical transition lines (the so-called structure plot) with the experimental data (open circles) as shown in figure 2. The occupied bulk band lines along the Γ–Λ–L direction display the results of nonlocal pseudopotential calculations [11]. The photon energies are evaluated assuming the free-electron-like final-state (FELFS) model via the following equation:

$$\hbar\omega = \frac{\hbar^2}{2m}(\boldsymbol{k}_\perp + \boldsymbol{G})^2 + E_b - V_0 \tag{1}$$

where the $\boldsymbol{k}_\perp$ is the momentum parallel to surface normal, $\boldsymbol{G}$ is the reciprocal-lattice vector of the crystal, and the inner potential $V_0$ was chosen to be 4.5 eV [9] which was most suitable for the present data. We consider that the valence band maximum is 0.18 eV below $E_F$ in this (2 × 2) surface where the Fermi level is assumed to lie at the bottom of the

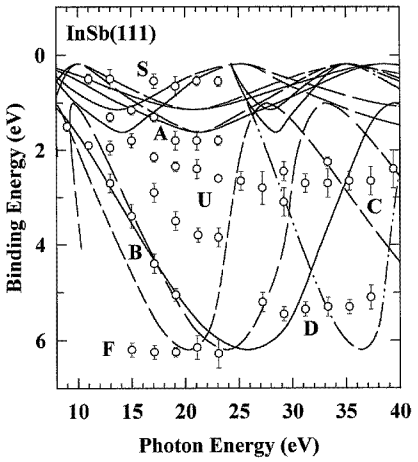


**Figure 2.** A structure plot for the normal-emission data for the InSb(111)–2 × 2 surface. The theoretical solid lines show early calculated results [11] and we assume the free-electron-like final state. Solid curves show direct transitions and the broken curves show secondary cone emissions. Open circles show the measured data, with error bars.

conduction band [9]. The solid curves represent direct bulk band transitions (primary cone emissions) while the other broken curves display secondary cone emissions scattered by other bulk $\boldsymbol{G}$-components such as $(2\pi/a)(1\bar{1}1)$, (200), and $(2\bar{2}0)$ sets where $a$ is the lattice constant [12]. The experimental bulk bands, labelled **A** and **B**, follow the solid curves which are attributed to the primary cone emissions. The weak feature **S** does not follow the dispersion of any theoretical line and shows no dispersion as the photon energy increases. In addition, it lies above the bulk valence band, i.e., in the bulk band-gap region. So, **S** is attributed to a surface state. The intensity of the surface state was expected to be as weak as those reported for GaAs(111) and InSb(111) surfaces while the other $(\bar{1}\bar{1}\bar{1})$ surface revealed many strong surface-state emissions [8, 13]. The dispersive states **U** do not seem to be related to the direct transitions from the bands of the Γ–Λ–L line. These are due not to the direct bulk emission but to the surface Umklapp process related to the surface $\boldsymbol{G}_{2\times2}$-vector, which allows the observed surface Umklapp transition starting at $(2\pi/a)(-1/3, -1/3, 2/3)$ and ending at $(2\pi/a)(1/6, 1/6, 7/6)$. The behaviour of **U** features assigned as the surface Umklapp emission is very similar to those of the GaAs$(\bar{1}\bar{1}\bar{1})$–2 × 2 surface [12]. The nondispersive features **C** and **F** are associated with the reflection of critical points at $\Sigma_1^{min}$ and $L_6$ respectively, as HH already pointed out in their studies [9, 14]. However, the feature **D** does not coincide with any critical point and it was not found before. It emerges at high photon energies and shows the maximum intensity as a major peak at $\hbar\omega = 31$–33 eV in figure 1(b). The value of this photon energy is close to the absorption edge of the Sb 4d core level. We also observed a typical resonance feature in the total yield spectrum (not shown here) in this region of photon energy. Therefore, **D** can be a resonance state, like the process

$$\text{Sb } 4d^{10}v^n \xrightarrow{\hbar\omega} \text{Sb } 4d^9v^n \rightarrow \text{Sb } 4d^{10}v^{n-1} \tag{2}$$

where v indicates a valence state of InSb. Because there is no Sb-derived unoccupied surface state or resonance in the present In-terminated (111) surface, this process is ascribed to the transition from the Sb 4d core level to an unoccupied state in the conduction band. The

state with the same binding energy was also reported for the InSb($\bar{1}\bar{1}\bar{1}$)–3 × 3 surface [13]. Thus, the **D** state is related not to the surface structure, but to a resonance state coupled with the Sb 4d core level.

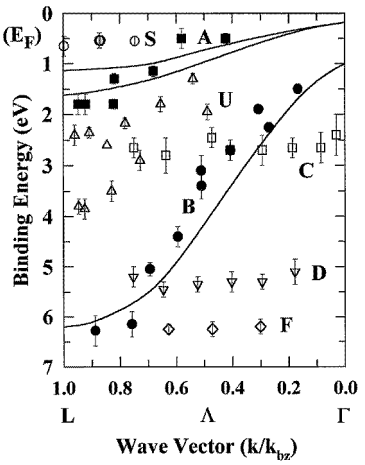


**Figure 3.** The measured band dispersion plot along the Γ–Λ–L⟨111⟩ direction in comparison with the theoretical results (solid line) [11]. Filled symbols show the direct bulk transition: **A** (square) and **B** (circle). Open symbols show the surface state (**S**: circle), the surface Umklapp emission (**U**: triangle), the resonance feature (**D**: inverted triangle), and the critical points (**C**: square and **F**: diamond).

The experimental energy bands in the reduced Brillouin zone (BZ) along the Γ–Λ–L direction are drawn together with the theoretical band calculation [11] in figure 3. Since $\boldsymbol{k}_{\parallel}$ is zero in normal emission, the perpendicular momentum component is calculated by assumption of the FELFS model using the formula

$$\boldsymbol{k}_{\perp} = \sqrt{\frac{2m}{\hbar^2}(\hbar\omega - E_b + V_0)} \pm \boldsymbol{G}_{\perp}. \tag{3}$$

$\boldsymbol{G}_{\perp}$ is the bulk reciprocal-lattice vector perpendicular to the surface. The band dispersions of **A** and **B** are in good agreement with the theoretical calculation, but others do not coincide with the theoretical lines. The dispersive bands **U**, which correspond to the surface Umklapp emission, show clear downward dispersion, like in the case of the GaAs($\bar{1}\bar{1}\bar{1}$)–2 × 2 surface [12]. The other nondispersive bands are shown at some region of restricted BZ. **C** and **F** are associated with the indirect transitions from the critical points of $\Sigma_1^{min}$ and $L_6$ respectively, as mentioned above. Other nearly flat features at $E_b = 0.6$ and 5.3 eV were not reported before and they do not match with any previously known bands. The band **S** at around $E_b$ = 0.6 eV is weak but appeared at low photon energies and lies near the BZ boundary above the bulk valence band. Therefore, we suggest that it is a true surface state delocalized on the surface forming the In back-bond-like state. Another band **D** at $E_b$ = 5.3 eV is dominant only at higher photon energy and lies within the bulk band. It is thought to be a resonance feature of this InSb(111)–2 × 2 surface even if the correct origin is not identified.

In summary, through the ARPES measurements of the InSb(111)–2 × 2 surface for normal-emission geometry we represented the bulk band dispersion along Γ–Λ–L⟨111⟩ direction. In addition to two bulk band transitions, we observed the surface Umklapp transition related to the reciprocal-lattice vector $\boldsymbol{G}_{2\times2}$. The bands at $E_b$ = 2.8 and 6.3 eV

are the indirect transitions from the high density of states of the bulk band structure. Newly observed flat bands at $E_b$ = 0.6 and 5.3 eV are the surface state and resonance state of this InSb(111)–2 × 2 surface, respectively.

## Acknowledgments

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