

## The structure of Sb(111) determined by photoelectron diffraction

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### Abstract

The Sb(111) 4d<sub>5/2</sub> core level is found to contain three components. Using photoelectron diffraction, these are assigned to photoemission from the first layer, the second layer and the bulk, respectively. The binding energy for the first and second layer atoms is found to be 120 meV lower and 330 meV higher than for the bulk atoms, respectively. As a by-product of this assignment, the geometric structure of the surface is determined. No substantial relaxations are found.

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The surfaces of the semimetals bismuth and antimony have recently attracted considerable attention, mainly due to their unusual electronic properties. All low-index surfaces studied so far turn out to be good two-dimensional metals [1–4] (for a review see Ref. [5]), in contrast to the bulk which is semimetallic with a very low density of states at the Fermi level [6]. Moreover, the two-dimensional surface electronic structure is strongly influenced by the spin-orbit splitting of the states [7,8].

A controversial point has been the nature of the shallow 5d core levels of Bi(111). Bi 5d<sub>5/2</sub> has been found to contain two components, separated by about 200 meV, which had been interpreted in terms of a surface core level shift (SCLS), such that the components with the higher and lower binding energies correspond to emission from bulk and first layer surface atoms, respectively [9]. A very different interpretation was later presented by Ast and Höchst [10] who argued that the low binding energy component is the principal core level peak line and the high binding en-

ergy component is caused by an energy loss. Later, the original interpretation was supported by a photoelectron diffraction experiment [11]; an approach which can be used to identify the origin of certain core level components [12,13].

In this paper, we present core level data from Sb(111). Surprisingly, and despite the otherwise great similarities of Bi(111) and Sb(111), the core level spectrum of Sb(111) shows three components instead of two. Using a large data set of angular photoelectron diffraction scans, we assign these components to emission from the first and second atomic layer and from the bulk. We also determine the geometric structure of Sb(111) which has not been reported previously.

The experiment was performed on the SuperESCA beamline of the storage ring ELETTRA in Trieste [14]. The angular resolution of the electron analyser was  $\pm 1^\circ$  and the combined energy resolution of beamline and electron analyser was in the order of 50 meV. The Sb(111) sample was cleaned by sputtering and annealing to 573 K. Cleanliness and surface order were ensured by X-ray photoemission spectroscopy and low energy electron diffraction (LEED), respectively. The surface showed a

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( $1 \times 1$ ) LEED pattern, as expected from earlier studies [15]. For all experiments, the sample was cooled to 185 K. So-called azimuthal scans were taken at different photon energies and polar angles  $\Theta$  (the polar angle is defined as the angle between the emission direction and the surface normal). The azimuthal scans were performed by rotating the sample around the surface normal. The electron analyser was mounted on the chamber under an angle of  $70^\circ$  from the incoming light, in the plane of polarisation. The intensities of the different components of the core level spectra were extracted using a curve fitting procedure (see below), as a function of azimuthal angle  $\phi$ . From the intensity curves  $I(\phi)$ , modulation functions were constructed according to  $\chi(\phi) = (I(\phi)/I_0) - 1$ , where  $I_0$  is the smooth part of  $I(\phi)$ . All modulation functions were found to be consistent with the three-fold symmetry axis perpendicular to the surface.

Fig. 1 shows three Sb  $4d_{5/2}$  spectra taken in normal emission ( $\Theta = 0^\circ$ ) at different photon energies. A consistent fit of these spectra, and the entire data set shown below, was possible by three components called C0, C1 and C2. All components were fitted with a Doniach–Sunjic lineshape [16] using a Lorentzian width of 270 meV, a Gaussian width of 207 meV and an asymmetry parameter of 0.01. The C1 and C2 components are separated from the C0 component by 120 meV and 450 meV, respectively. Fig. 2 shows the integrated intensity for these three components for three scans of the azimuthal angle at a photon energy of  $\approx 146$  eV and polar emission angles of  $45^\circ$ ,  $55^\circ$  and  $65^\circ$ . The inset of Fig. 2 gives the truncated bulk geometric

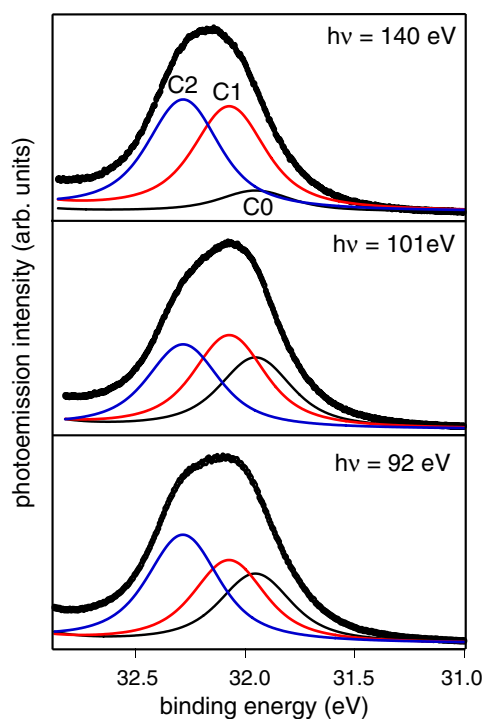


Fig. 1. Sb  $4d_{5/2}$  spectra taken in normal emission at different photon energies.

structure of the surface. The top view of the surface shows hexagonal close-packed planes and the side view shows the characteristic bilayer stacking of the group V semimetal structure. Pseudo-covalent bonds are indicated as solid lines [15].

Already from an inspection of Figs. 1 and 2, the component C0 can tentatively be assigned to emission from the first atomic layer. The first reason for this is its suppression at higher photon energies where the inelastic mean free path of the electrons increases, and its enhancement at higher off-normal emission angles where the experiment is more surface sensitive. The second reason is the weak modulation, compared to that of the other curves. Relatively weak modulations are expected for the first layer because of the absence of forward scattering by atoms above the emitter, a strong effect in angle-scan photoelectron diffraction [17]. The other components C1 and C2 do indeed show the characteristic sign of forward scattering at azimuthal emission angles of  $\phi = \pm 60^\circ$  (forward scattering should occur for a polar emission angle around  $58.5^\circ$ ). Note, however, that the latter argument has to be used with some care. While the modulus of the forward scattering factor is dominant at all energies, the scattering phase shift is not necessarily zero for low energies. In extreme cases this can lead to a suppression instead of an enhancement in the forward scattering direction. Finally, the similarity of Sb(1 1 1) and Bi(1 1 1) suggests that the lowest binding energy component corresponds to the outermost layer [9,11]. From a mere inspection of the azimuthal scans, it is not obvious how to assign the C1 and C2 components. In any event, a firm proof of the correct assignment must come from comparison with multiple scattering calculations.

Photoelectron diffraction calculations were performed using the numerical code developed by Fritzsche [18,19]. This code uses an expansion of the scattering processes into scattering paths [20]. The successive scattering events on a scattering path are treated within a Green's function formalism using a magnetic quantum number expansion for the free electron propagator [21]. Multiple scattering was included up to triple scattering. The cluster for the calculations was modelled as a six layer tall cylinder with a radius of  $30 \text{ \AA}$  on top of a hemisphere, also of  $30 \text{ \AA}$  radius. We have used  $L_{\text{max}} = 18$  scattering phase shifts. The inelastic mean free path was modelled by the universal curve [22]. These parameters were not systematically optimised but rather represent a conservative choice. Tests have shown that none of the results reported below depend critical on the detailed values of the parameters.

As a starting point for the surface structure, we used the truncated bulk shown in Fig. 2. In principle, the surface could be terminated with a broken instead of an intact bilayer but this termination is unphysical and was not considered. Modulation functions were extracted from the calculated intensities and compared to the experimental modulation functions using the reliability factor  $R_M$  which measures the square deviations between experimental and theoretical diffraction curves [23].

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