ELSEVIER

Physica B 198 (1994) 243–245

PHYSICA B

X-ray structure analysis of the InSb $(\bar{1}\,\bar{1}\,\bar{1})$-$(3 \times 3)$ reconstruction

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Abstract

The (3×3) reconstruction of the InSb $(\bar{1}\,\bar{1}\,\bar{1})$ surface has been analysed using grazing incidence X-ray diffraction. The reconstruction is characterized by hexamers above a complete InSb double-layer centred around an Sb atom. No vacancies are found in the structure as predicted theoretically. The results agree with scanning tunnelling microscopy measurements.

Results and discussion

The $(\bar{1}\,\bar{1}\,\bar{1})$ surface of InSb is terminated by Sb atoms and has a (3×3) reconstruction. In contrast to the In terminated (1 1 1) surface which has a (2×2) reconstruction [1] little is known about the atomic structure of this polar surface. From total energy calculations [2] no vacancies are expected which have been observed for InSb (1 1 1) (2×2) and GaAs (1 1 1) (2×2) [3].

The InSb $(\bar{1}\,\bar{1}\,\bar{1})$ surface was prepared in UHV by Ar^+ ion bombardment and annealing at 673 K for about 3 h followed by slow cooling to room temperature (2 K/min). The data were collected at the W1 wiggler beam line at the Hamburger Synchrotron Strahlungs Laboratory (HASYLAB) at an X-ray incidence angle of $\alpha_i = 1.0°$ and an X-ray wavelength of $\lambda = 1.316$ Å. The data set consists of 278 independent reflections, corresponding to 71 in-plane superlattice reflections $(q_\perp = l \times c^* \approx 0)$ and to 24 superstructure lattice rods measured up to a maximum momentum transfer normal to the sample surface, $q_\perp = 0.64$ Å^{-1}.

The large out-of-plane dataset was essential for deriving an unambiguous structure model since it allows the calculation of Patterson sections. The Figs. 1(a) and 1(b) show the Patterson functions calculated on the basis of the $q_\perp = 0$ dataset and the dataset including the $q_\perp \neq 0$ reflections, respectively. Correspondingly, Fig. 1(a) shows the Patterson function projected along z, the coordinate normal to the sample surface. In contrast, in Fig. 1(b) the section $P(u\,v\,0)$ is shown where two (positive) interatomic vectors are indicated by 1 and 2. Additional maxima are also observed and they will be discussed elsewhere [4]. The interpretation of these vectors was the key for solving the structure.

The (in-plane) vectors observed in the $P(u\,v\,0)$ function can be related to interatomic vectors within a six-membered ring shown in Fig. 2. The assignment of the atoms to In and Sb was made on the basis of the bonding angles (sp^2 hybridization of In and p-type bonding of Sb). The whole structure on the basis of the best fit to the measured data ($R_w = 0.045$, GOF = 1.09) is shown in Fig. 3. A different ring structure has been determined for the $(\sqrt{19} \times \sqrt{19})$ surface of GaAs from STM measurements [5].

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SSDI 0921-4526(93)E0547-T

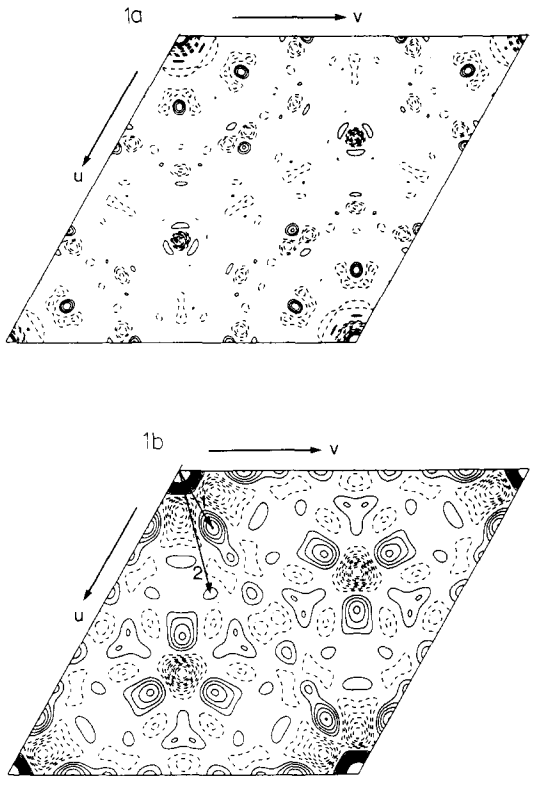

Fig. 1. Projected Patterson-function of the (3 × 3) reconstruction (a) and Patterson section $P(uv0)$ (b). Two in-plane interatomic vectors (1–2) of the six-membered ring are indicated (see e.g. Fig. 2) in the section which do not appear in the projection. Since only fractional order reflections are used negative maxima also appear and they are shown as dashed lines.

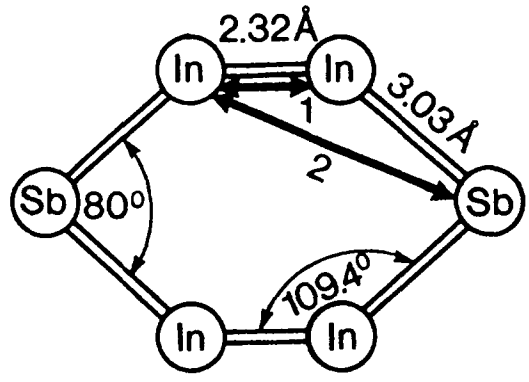

Fig. 2. Six-membered ring of In and Sb atoms. Two interatomic vectors observed in the Patterson section $P(uv0)$ are labelled by 1 and 2.

The six-membered rings are located above a complete InSb double layer. The rings are centred around an Sb atom. Besides these rings having 2 mm symmetry a small fraction (≈ 0.07) of trigonal rings is present. The results agree well with STM measurements [6] indicating the presence of "elliptic" and trigonal structure elements above the top layer. The elliptic and trigonal rings can be arranged in three and two orientations, respectively. From the bond angles within the rings, orbital rehybridization of the constituent atoms and depolarization of the surface are found to be one of the important characteristics

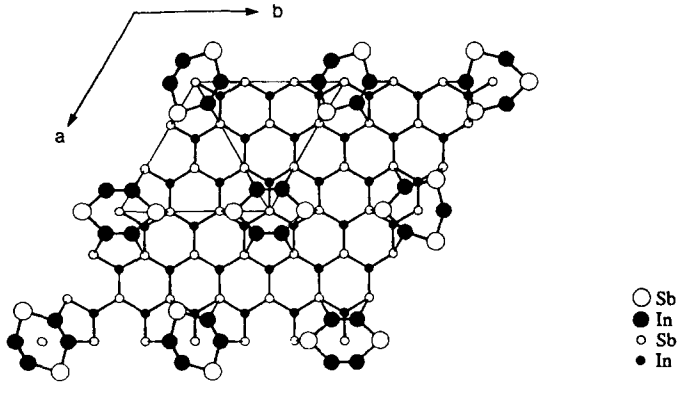

Fig. 3. Structure model of the (3 × 3) reconstruction of InSb ($\bar{1}\,\bar{1}\,\bar{1}$). One 3 × 3 unit cell is indicated by the solid lines. Two types of six atom rings are located above the top layer. The rings are centred around an Sb atom.

of the surface structure. This is in correspondence to the (2×2) reconstruction. However, in this case rehybridization is made possible by creation of a vacancy and inward relaxing of the InSb double layer [1].

In contrast to only small in-plane atomic displacements (at most 0.1 Å) significant relaxations were found along the normal direction. The orientations of the rings have no notable influence on the relaxations within the underlying double layer.

Temperature dependent measurements of the (1/3 0) superlattice reflection indicated a reversible phase transition $(3 \times 3) \rightarrow (1 \times 1)$ at 648 K. A hysteresis is found suggesting a first-order transition which is expected from symmetry considerations.

Acknowledgement

The support of this work by the Bundesministerium für Forschung und Technologie under grant #05464IAB8 is gratefully acknowledged.

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