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Core level photoemission from (111)-type InAs surfaces

C.B.M. Andersson, L.Ö. Olsson*, M.C. Håkansson**, L. Ilver*, U.O. Karlsson and J. Kanski*

Department of Physics, Royal Institute of Technology, 100 44 Stockholm, Sweden

** Department of Physics, Chalmers University of Technology, 430 40 Göteborg, Sweden*

*** Department of Synchrotron Radiation Research, University of Lund, 223 62 Lund, Sweden*

ABSTRACT

The InAs(111)2x2 and InAs($\bar{1}\bar{1}\bar{1}$)1x1 surfaces have been studied with high resolution core level spectroscopy. For the InAs($\bar{1}\bar{1}\bar{1}$)1x1 surface both the In 4d and the As 3d core levels display strong surface core level shifts, while for the InAs(111)2x2 surface only the In 4d level shows a detectable surface shift. The results indicate that the InAs($\bar{1}\bar{1}\bar{1}$)1x1 surface is relaxed, with atom layer displacement extending to subsurface layers. Unexpectedly, we find no surface shifted anion core level for the InAs(111)2x2 surface.

1. INTRODUCTION

The atomic and electronic structure of the polar (111) surfaces of III-V semiconductors have gained an increased attention during recent years [1-8]. Depending on crystal orientation and stoichiometry, the (111)-type surfaces display different atomic geometries. The most common reconstruction for the clean (111) surface is 2x2, as seen in low energy electron diffraction (LEED), while the ($\bar{1}\bar{1}\bar{1}$) surface displays several reconstructions as function of surface composition.

In this paper we report results from high resolution core level spectroscopy studies of the InAs(111)2x2 and InAs($\bar{1}\bar{1}\bar{1}$)1x1 surfaces. Since different geometrical configurations are reflected via different binding energies, core level spectra can be utilized to provide direct information about the presence of inequivalent surface sites and their relative abundance. In this way core level spectroscopy serves as an important complementary tool for structural determinations. Increased knowledge about the surface geometries for the clean surfaces may be significant for utilizing InAs in high-speed electronic-device applications, since the formation of high quality heteroepitaxial interfaces are of supreme importance in such devices.

2. EXPERIMENTAL

The experiments were performed at the toroidal-grating monochromator beam line at the MAX synchrotron radiation facility in Lund, Sweden [9]. The angle resolved photoelectron spectra were recorded

with a modified VSW ARIES system. Interlocked with the photoemission system is a molecular beam system equipped with six effusion cells and RHEED.

The InAs substrates were sulphur doped and were supplied by MCP Wafer Technology Limited, England. The InAs($\bar{1}\bar{1}\bar{1}$)1x1 and the InAs(111)2x2 surfaces were prepared by repeated cycles of sputtering and annealing. This preparation procedure yielded well ordered surfaces, which showed sharp LEED patterns with a low background. Both surfaces could also be grown by MBE, and showed the same photoemission spectra.

3. RESULTS AND DISCUSSION

Figure 1a shows In 4d and As 3d spectra from the InAs(111)2x2 surface measured at 0° and 60° emission angles, i.e. at different surface sensitivities. Also shown in the figure are decompositions into spin-orbit split Voigt functions. The fitting parameters are given in Table 1. It is seen from the figure that the In 4d spectra can be constructed from two different components, while only one component is necessary for the As 3d core level. From the intensity variations between the two In 4d components as function of emission angle and photon energy it is clear that the component towards higher binding energy is surface related.

In figure 1b the In 4d and As 3d core levels from the InAs($\bar{1}\bar{1}\bar{1}$)1x1 surface are displayed together with the corresponding decompositions. From the raw data it is clearly seen that both the In 4d and the As 3d spectra are broader than the corresponding spectra from the InAs(111)2x2 surface. A deconvolution based on similar parameters as used for the (2x2) surface shows that at least two components are needed to adequately fit the experimental data. For the As 3d level we note that both components have about the same intensity independent of emission angle. The identification of the As 3d bulk component was accomplished by increasing the photon energy and thereby the bulk sensitivity. Additionally, we have used the established separation between the In 4d and As 3d bulk components. The lack of an intensity enhancement of the surface component as function of emission angle may be due to diffraction effects, which are known to be strong in this energy range from III-V semiconductors [11]. These effects could in principle be used for a geometrical structure determination. This would, however, require substantially more data on the angle- and energy dependence.

Figure 1 Core level spectra from the InAs(111)2x2 and InAs($\bar{1}\bar{1}\bar{1}$)1x1 surfaces. In each case the dots represent the experimental data, while the lines show the fitted curves.

The (111) surfaces of III-V semiconductors have been subject to extensive experimental and theoretical studies. Based on LEED investigations Tong et al. proposed a vacancy-buckling model for the GaAs(111) surface with one of four surface gallium atoms missing [1]. Robinson et al. studied the InSb(111)2x2 and GaSb(111)2x2 surfaces by X-ray diffraction and found that the vacancy-buckling model could well explain the experimental data if the distortions were permitted to extend down to the second layer [4]. The vacancy model for the (111)2x2 surfaces was given further support when Haberern and Pashley could resolve individual surface gallium atoms in their scanning tunneling microscopy images of the GaAs(111)2x2 surface [5].

	InAs(111)2x2				InAs($\overline{1}\overline{1}\overline{1}$)1x1			
	In 4d		As 3d		In 4d		As 3d	
	0°	60°	0°	60°	0°	60°	0°	60°
s-o splitting	0.855	0.855	0.685	0.685	0.855	0.855	0.685	0.685
branching ratio	1.18	1.37	1.52	1.54	1.23	1.29	1.58	1.47
surface shift	-0.27	-0.29	—	—	-0.29	-0.29	0.27	0.27
surface/bulk intensity ratio	0.72	2.69	—	—	0.23	0.91	1.77	1.58
$\Delta E_{\text{Gaussian}}$	0.33	0.38	0.40	0.40	0.41	0.40	0.40	0.40
$\Delta E_{\text{Lorentzian}}$	0.175	0.175	0.16	0.16	0.175	0.175	0.16	0.16

Table 1 Fitting parameters for core level spectra from InAs(111) 2x2 and InAs($\overline{1}\overline{1}\overline{1}$)1x1 surfaces. The Lorentzian was kept constant in the fitting process.

Given the similarities in the atomic and electronic structure for the other III-V surfaces it is likely that the vacancy model should apply also for the InAs(111)2x2 surface. This is partly in agreement with our core level spectra. In the vacancy-buckling model for the 2x2 reconstruction the surface group III and group V atoms are rearranged in such a way that the surface geometry locally is reminiscent of the non-polar (110) surface. Disregarding possible differences in the final state one would therefore expect the surface core-level shifts to be similar to the shifts measured for the (110) surface. For the In 4d core level this is indeed the case. The present results show a surface core level shift of 0.28 eV, which is similar to the 0.27 eV found for the (110) surface [10]. In the case of As 3d, however, the situation is quite different. On the (110) surface the As 3d level displays a surface shift of 0.30 eV [11], but on the (111)2x2 surface we can not resolve any shifted component - the As 3d line shape is independent of emission angle and the spectrum is well fitted with a single component. A similar result is obtained on the corresponding InSb surface[12]. Considering, in addition, that the vacancy-buckling model includes two types of surface anion sites, namely the three anions which surround a vacant cation site and a single anion, not adjacent to any vacancy site, the absence of any significant shifted As 3d component in the present spectra is surprising. Our observation may possibly be understood on the basis of charge density calculations by Kaxiras et al. [3]. Within the vacancy-buckling model these authors found that the three As atoms around the vacancy site relax toward this site and attain an almost p^3 bonding configuration. Furthermore, the single As atom which is not adjacent to any vacancy site could also be assumed to attain a p^3 bonding configuration. It could then be argued that the local charge arrangement at the surface anions is rather similar to that in the bulk, and consequently, the surface core level shifts would be very small. It is then also assumed that all other effects which contribute to

surface shifts (Madelung potential, final state screening) are either similar to the corresponding bulk properties, or tend to cancel each other. Clearly, further studies of this phenomenon are of interest.

Several III-V (111) surfaces display a 1×1 LEED pattern [6-8]. Hou et al. studied the $\text{InP}(\bar{1}\bar{1}\bar{1})1 \times 1$ surface by angle resolved photoelectron spectroscopy and compared the experimentally obtained dangling bond dispersion with a theoretical calculation based upon a slab model and the extended Hückel theory [6]. The results showed that the $\text{InP}(\bar{1}\bar{1}\bar{1})1 \times 1$ surface is a relaxed surface with the atomic layer displacement extended to the outermost four layers. The dangling bond dispersion found by Hou et al. for the $\text{InP}(\bar{1}\bar{1}\bar{1})1 \times 1$ surface is very similar to dangling bond dispersion for the $\text{InAs}(\bar{1}\bar{1}\bar{1})1 \times 1$ surface [8]. This indicates that also this surface exhibits a displacement of the subsurface atoms. It is therefore likely that both the In and the As should show surface shifted components, in good agreement with our experimental observations.

4. SUMMARY

Surface sensitive high resolution core level spectroscopy has been applied to the $\text{InAs}(111)2 \times 2$ and $\text{InAs}(\bar{1}\bar{1}\bar{1})1 \times 1$ surfaces. For the $\text{InAs}(\bar{1}\bar{1}\bar{1})1 \times 1$ surface both the In 4d and the As 3d core levels displayed strong surface core level shifts, while for the $\text{InAs}(111)2 \times 2$ surface only the In 4d level showed a detectable surface shift. The results indicate that the $\text{InAs}(\bar{1}\bar{1}\bar{1})1 \times 1$ surface is a relaxed surface with atom layer displacement extending to subsurface layers. For $\text{InAs}(111)2 \times 2$ no surface shifted As core level is detected, which may possibly be due to similar local charge density on the surface anions as in the bulk.

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