Giant band bending and interface formation of Cs/InAs(110) at room temperature

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Abstract: We show by synchrotron radiation core level photoemission spectroscopy that minute amounts of Cs induce at room temperature a giant jump of the Fermi level into the conduction band when deposited on well-cleaved InAs(110) surfaces. This stage corresponds to a single Cs adsorption site. When more Cs is added a new adsorption site appears while correlatively the band bending gradually decreases. The complete interface formation (electronic structure, chemistry) is followed up to saturation at one monolayer and analyzed in terms of the present models of Schottky barrier formation.

1. INTRODUCTION

During the last years it was established and confirmed in different experiments that upon deposition of minute amounts of noble metal atoms at ~ 20 K onto InAs(110) cleaved surfaces one induces a large movement of the Fermi-level (E_F) well into the conduction band (see, e.g., [1]). Very recently in [2] was shown by synchrotron radiation core level photoemission spectroscopy (SRPES) that the deposition of small amounts of Cs on the InAs(110) surfaces induces already at room temperature (RT) and even deeper movement into conduction band thus creating probably the highest E_F pinning position (~ 0.6 eV) above the conduction band minimum (CBM) ever met for a semiconductor. In this paper we present detailed investigation of this phenomenon. We will show that the giant jump of the Fermi level into the conduction band which takes place at very low Cs coverages corresponds to a single Cs adsorption site. With further Cs deposition a new adsorption site appears while correlatively the band bending gradually decreases. The complete interface formation (electronic structure, chemistry) is followed up to saturation at about one monolayer and analyzed in terms of the present models of Schottky barrier (SB) formation.

2. EXPERIMENTAL DETAILS

The photoemission measurements were performed on the Mark II grasshopper monochromator beam line at the "Aladdin" 1 GeV storage ring of the University of Wisconsin-Madison. The photoelectron energies were analyzed by an angle-integrating double-pass cylindrical mirror analyzer at a working pressure around $3 - 4 \times 10^{-11}$ Torr. The typical instrumental resolution was ~ 0.25 eV. Clean InAs(110) surfaces were obtained by in-situ cleaving of InAs single crystals having doping concentrations $\approx 3.10^{17}$ cm⁻³ for both p-type (Zn doped) and n-type (S doped) samples. Pure Cs was deposited at RT onto the InAs(110) surfaces using an extremely well outgassed SAES source (typically during Cs deposition the maximum pressure rise did not exceed 2×10^{-11} Torr). To achieve the best accuracy in the band bending measurements, we have always kept the same photon energy (122 eV or 90 eV) to avoid any potential problem with the photon energy reproducibility and have never moved the monochromator within a specific series of measurements. We have also measured the work function changes upon Cs deposition from the low-energy cutoff shifts in the photoemission spectra, monitored with a ~ 7 V sample bias. Other details concerning data acquisition and alkali metal deposition can be found elsewhere (see, e.g., [1-3]).

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3. RESULTS

Fig. 1 displays the evolution of the In 4d and As 3d core levels at increasing Cs amounts deposited onto the RT p-InAs(110) surface. The photon energy was 122 eV. Due to the space limitation here we can not display the result obtained for n-type samples as well as those for 90 eV photon energy. However they show similar evolution and will be published in other paper. For the same reasons we do not show here the results of the fitting procedure of these spectra.

Fig. 1. In 4d (a) and As 3d (b) core-level normalized spectra of the Cs/p-InAs(110) interface at RT for increasing Cs coverages.

Fig. 2. (a): Cs 4d core-level photoemission spectra of the Cs/p-InAs(110) interface at RT for increasing Cs coverages. The spectra correspond to the same series of depositions and measurements as those in Fig. 1. All spectra are normalized to equal height. (b): The results of Cs 4d core-level decomposition for the data presented in Fig. 2a (first seven spectra with coverages 0.01-0.25 ML). Scale factors are indicated. The solid lines are the results of a least-squares fitting procedure, a polynomial background function and the sum of the three previous contributions.

The deposition of small amounts of Cs causes a very strong shift of the In 4d as well as As 3d spectra to lower kinetic energy. This shift reaches the maximum (~ 0.8 eV) at around 0.03 - 0.05 ML and decreases with further coverages. Even using just this row data of these In 4d and As 3d core levels one is able to measure precisely enough the value of the corresponding downward band bending versus Cs coverages and therefore derive the E_F position changes at the surfaces for both p- and n-type substrates.

In Fig. 3 we present Cs 4d core-level photoemission spectra of the Cs/p-InAs(110) interface at RT for increasing Cs coverages. The spectra correspond to the same series of depositions and measurements as those in Fig. 1. In Fig 3(b) we show the Cs 4d core-level decomposition results for the data presented in Fig. 2a (first seven spectra with coverages 0.01 - 0.25 ML). The spectra are fitted with 2 spin-orbit split doublet components C and D (fitting parameters: spin-orbit splitting 2.3 eV; branching ratio 1.4; Lorentzian FWHM 0.35 eV; Gaussian FWHM 0.6 - 0.7 eV; instrumental resolution 0.35 eV; polynomial background).

Fig. 3. Fermi level position at the InAs(110) surfaces for p- type (open symbols) and n-type (closed symbols) samples as a function of Cs coverages at RT. The circles and triangles correspond to data, obtained from the bulk component shifts of the In4d and As3d core levels respectively.

It is clear, even from direct visual inspection, that at very low coverages only one C component is detectable. However starting from ~ 0.02 ML one can distinguish another component, D, at lower binding energy. Its relative intensity is growing with coverage and becomes larger than the first one at about 0.25 ML. The two doublet components are separated by about $\Delta E \sim 1.0$ eV. Similar doublets for other Cs/A³B⁵ systems in the submonolayer regime were observed in refs. [3, 4], but not in ref. [5]. This splitting could indicate that two inequivalent adsorption sites having a large difference in ionicity exists for the Cs adatoms at InAs(110) surface in this range of coverages (0 - 0.25 eV). However there could be and other explanations: e.g., the C component could correspond to single Cs atoms adsorbed on the InAs(110) surface, while the second component could originate from dimers, trimers etc..., as proposed for the Na/GaAs(110) system in ref. [5].

3. DISCUSSION

We first follow the E_F motion at various Cs coverages using the In 4d and As 3d core levels. Fig. 1 shows as example the evolution of the In 4d and As 3d core level spectra deposition of Cs onto the p-InAs(110) surfaces at RT. From the core-level energy shifts for both p- and n-type substrates, one derives the E_F position changes at the surfaces versus the Cs coverages. Since the initial kinetic energy difference between the In 4d (as well as the As 3d) core levels for the clean surfaces of our n- and p-type samples was 0.25 - 0.30 eV, flat band conditions were met in our experiments. Consequently we can conclude that the initial E_F positions at the clean cleaved surfaces were the same as in the bulk. Hence Fig. 3 shows the surface E_F positions relative to the fundamental gap edges versus the Cs coverages (for p- and n-type

samples). One can observe that, upon RT deposition of such low Cs coverages as ~ 0.01 - 0.02 ML, the E_F position at the (110) surfaces for p- and n-InAs(110) dramatically depends on the coverage: it jumps to an extremely high position and reaches its maximum (about 0.6 eV above the CBM) already at 0.03 - 0.05 ML Cs. This E_F position is probably the highest pinning position above the CBM ever observed on a semiconductor surface. This movement corresponds to a very large downward band bending and suggests the creation of a two dimensional electron gas at the surface. With further Cs deposition the E_F position at the surface decreases and reaches a value about 0.2- 0.3 eV above CBM.

To our knowledge, there is so far no theoretical publications on the metal adatoms-InAs(110) interaction. However the results presented here can be explained by analogy with other Cs/ A^3B^5 systems, [3, 5 - 10]. At very low coverage the Cs atoms are likely to stay apart or form linear chains as observed on other A^3B^5 compounds [11] and to create donor type surface states. The position of the donor type metal adatom induced surface states can be identified at the maximum of the E_F positions at very low Cs coverages (Fig. 3). Again referring to theoretical calculations for alkali metals and other s electron like metals (Ag and Au) [6 - 10], one can relate this donor state to the Cs - In bonding state located above the CBM and filled when the surface is neutral. The presence of this donor type level above the CBM explains the band bending behavior versus coverage for both p- and n-type substrates. Electrons are donated from this level to the semiconductor bulk, producing a positive surface charge which leads to a huge downward band bending.

These conclusions are in good agreement with our results, presented in Fig. 2. In the very low coverage regime we observed only one Cs 4d component, which was growing with coverage. Most probably this indicates that these Cs atoms preferentially bond to the In atoms in a rather ionic type of bonding and transfer its valence electron to the In empty dangling bond (at least in part). In the same coverage regime we observed that huge band bending. When the second Cs 4d component, D, appears the band bending increases more slowly and stops when both components are reach nearly the same intensity at about 0.03 - 0.05 ML. The decrease of the BB correlates with the relative increase of the second Cs 4d component.

At the end of this short report, we should discuss the reactivity of the InAs(110)system. In [4,5] it was shown that Cs has no reaction with the GaAs(110) surface and further in ref. [6] it was indicated, that the InAs(110) surface is more inert than the GaAs(110) one. Therefore one could think, that Cs has no reaction with InAs(110) surface as well. However, the In 4d and As 3d spectra in Fig. 1 show very strong reactive components at coverage ≥ 0.5 ML.

5. CONCLUSIONS

In the present work we show that E_F can move at room temperature to an extremely high pinning position above the CBM, up to ~ 0.6 eV for Cs/InAs(110), which distinguishes very significantly this semiconductor from any other ones. The existence of only one adsorption site at the same coverages, were we observed such a huge band bending, proves that this BB is the consequence of the bonding of the Cs atoms to the In ones and the creation of donor type surface states placed nearly ~ 0.6 eV above CBM. The Fermi level pinning at this very high position above the CBM strongly suggests the existence of a two-dimensional electron gas at the surface.

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