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Giant band bending induced by Ag on InAs(110) surfaces at low temperature

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We show by synchrotron radiation photoemission spectroscopy [G. Le Lay, V. Yu Aristov, J. Kanski, P. O. Nilsson, U. O. Karlsson, K. Hricovini, and J. E. Bonnet (unpublished)] (core levels and valence band) as well as by Kelvin probe measurements, both under illumination and in the dark, at low temperature (LT) $T \approx 20$ K and room temperature (RT) $T \approx 300$ K, that upon deposition of minute amounts of silver (about 0.01–0.1 monolayer) onto *in situ* well-cleaved, highly doped, *n*- and *p*-type InAs(110) surfaces, one induces a giant movement of the Fermi level E_F into the conduction band. We thus create a two-dimensional (2D) electron gas at the surface (strong downwards band bending): as a matter of fact, we do observe emission of electrons from filled states up to the E_F placed far above the conduction-band minimum (CBM). It is also shown that the growth is laminar at LT, while it follows a Volmer-Weber mode at RT, with indications of chemical interactions between the Ag and In atoms at both temperatures. At LT the deposited atoms interact with the dangling bonds of the In atoms and saturate them for $\theta \approx 1$ monolayer (ML). At low coverages and LT, the individual Ag atoms create donorlike surface states (SS) (adsorption-induced states) and E_F can be pinned by these SS in the conduction band. This leads to the formation of a 2D electron channel at the InAs surface already at $\theta \approx 0.01-0.1$ ML for both types of semiconductors. At higher coverages one observes the onset of metallization for both temperatures and Ag clusters can produce another type of SS, typically metal-induced gap states near the CBM. These proposals, as well as the experimental facts, are discussed in the light of the current theoretical models of Schottky-barrier formation.

I. INTRODUCTION

There is a huge amount of experimental works devoted to the difficult study of metal-semiconductor (*M-S*) interface formation. These studies are extremely important both from the theoretical point of view and for solid-state device technology. Yet until recently this problem appeared very complicated. Employing low temperatures, $T \leq 80$ K, resulted in marked progress in the understanding of *M-S* interface formation. Now it is clear that the E_F position at a *M-S* interface, which is responsible for the electronic properties of the interface, has strong correlation with the interfacial atomic structure.

Roughly speaking, the deposited metal atoms might be in two different states on the substrate depending on the adsorption conditions. It is established that upon RT deposition at least the noble metals form three-dimensional (3D) metallic islands on $A^{III}B^{V}$ semiconductor substrates from the very initial stages of adsorption and the semiconductor surface between the islands remains clean:[1–7] this is the Volmer-Weber (VW) growth mode. In this case the decay of the wave functions of the metallic islands into the semiconductor band gap between the valence-band maximum (VBM) and E_F produces the so-called metal-induced gap states (MIGS),[8–11] that are mainly responsible for E_F pinning at RT deposition. During deposition of the same metals onto substrates at low-temperature (LT) the condensed atoms stay apart[12–14] and one observes a quite different behavior of E_F positioning. For example, on GaAs, in the submonolayer coverage region, the metallic atoms stay isolated and produce donor-type adsorption-induced states (AIS),[15] where E_F can be fixed. A few papers were devoted to the calculations of these AIS for different metal/GaAs(110) systems.[16–18] Therefore one can see that the conditions of metal deposition may play a crucial role in the electronic structure formation at the interface at the same stages of metal adsorption. Nevertheless at the surface E_F moves usually upon metal deposition inside the gap of GaAs.

However, a very unusual behavior is obtained for adsorbate-InAs systems. A few previous studies of clean and adsorbate covered InAs surfaces[19–25] have given some indications of the possibility of movement of E_F into the conduction band (and in the case of oxygen adsorption even proved it[21]). This movement might create a 2D electron gas at the surface [strong downwards band bending (BB)].

In this work we have studied the initial stages of the Schottky-barrier (SB) formation for the Ag/InAs(001) system. We prove that upon deposition of a very small amount of silver onto *in situ* well-cleaved InAs(110), adsorbed metallic (Ag) atoms induce donor-type AIS well above the conduction-band minimum (CBM). As a result, one observes a giant movement of E_F well into the conduction band and therefore the creation of a 2D electron channel at the surface. Using synchrotron radiation photoelectron spectroscopy (core levels and valence bands), as well as contact potential, difference measurements we establish undoubtedly its existence.

II. EXPERIMENTS

The InAs(110) surfaces were obtained by cleaving in the analytical chamber with base pressure 5×10^{-11} Torr. Only high-quality cleavages with flat bands were studied. Ag was evaporated from a preoutgassed, resistively heated, tantalum wire basket at a very small rate. The deposition rate was calibrated before and after each experiment with a quartz thickness monitor placed very close to the sample. Coverages θ are expressed in ML ($\theta=1$ ML corresponds to one Ag atom per substrate surface atom, i.e., 7.75×10^{14} atoms/cm^2). The total pressure of the residual gases during deposition was less than 2×10^{-10} Torr, otherwise at RT less than 1×10^{-10} and at LT 5×10^{-11} Torr.

It is well known that photoemission data can be affected by light as well as by synchrotron radiation illumination (surface photovoltage effect—SPV)[26–33] so one should pay attention to this possibility. InAs is a narrow gap (≈ 0.36 eV at RT) semiconductor which has a very small effective mass of electrons. As a result of that, the doping impurities are extremely shallow (≈ 3 meV). Therefore there should not be any SPV even at LT. Nevertheless to avoid any possible SPV even on this small gap semiconductor we have chosen highly doped, nearly degenerated, n- and p-type samples: dopant concentrations $n\approx3\times10^{17}$ cm^{-3}) (S), $p\approx6\times10^{17}$ cm^{-3} (Zn); mobilities $m_n\approx1.5\times10^4$ cm^2 V^{-1} s^{-1} at RT, 1.9×10^4 cm^2 V^{-1} s^{-1} at liquid-nitrogen temperature (LNT); $m_p\approx1.8\times10^2$ cm^2 V^{-2}s^{-1} at RT, 1.0×10^2 cm^2 V^1 s^{-1} at LNT. We have checked that the core-level (CL) peak positions were independent on the temperature between 20 K and LNT both upon heating and cooling.

However to check further that there is no SPV effect at all, we have carried out two types of experiment. First of all, we have reduced the photon intensity by more than ten times without noticing any influence. However we did not try to compare the energy position of the metallic step arising from metal deposition at the very early stages of its observation with reference to a gold sample metallic step at different illuminations, because our main effects were observed at $\theta\approx0.01-0.1$ ML (much before any metallic step formation). Our second type of experiments to check the possible influence of some SPV was carried out using Kelvin probe measurements, both under illumination and in the dark, at LT and RT. For this we used a vibrating electrode made from a gold grid in the form of a very thin plate of about 3 mm diameter. This plate was placed parallel to the surface studied very close to it. The vibration frequency was 182 Hz and the vibration amplitude a few tenths of a micrometer. The alternating current was measured by using a lock-in technique. We borrowed this Kelvin probe tool from Professor Chiaradia and used his methodology.[29] A more detailed description of a similar methodology can be found in Refs. 30–32.

The photoemission experiments were carried out at the SU6 beam line of the SuperACO storage ring at Laboratoire Pour l'Utilisation du Rayonnement Électromagnetique Orsay, France. Typical total instrumental resolutions were kept below 0.3 eV. All spectra were recorded at normal emission (2° acceptance angle).

III. METHODOLOGY FOR CORE-LEVEL ANALYSIS

The In4d and As 3d core-level spectra were analyzed following our standard rigorous methodology[31–34] using least-squares curve fitting. The parameters are summarized in Table I. The spin-orbit splitting and Lorentzian width (lifetime) of each core level were kept as fixed parameters. Again to minimize the number of free parameters we constrained the same values for the Gaussian widths of the bulk and surface components in the In 4d and As 3d spectra. Indeed the Gaussian widths are broader at RT as compared to LT due to phonon broadening. Doniach-Sunjic asymmetric line shapes were included because of metallic screening for Ag coverages corresponding to the appearance of metallicity (emission at E_F).

IV. GROWTH MODE

It is well known[1–7] that at RT noble metals grow in form of 3D metallic islands, following the VW mode (the surface of the substrate keeps clean metallic islands) during deposition onto $A^{\mathrm{III}}B^{\mathrm{V}}$ compounds at submonolayer coverages. From the other side the absorption of metal atoms onto a cold ($T\approx20$ K) substrate is characterized by a high rate of cooling of the deposited atoms because their hopping frequency is drastically quenched.[12,13] Moreover, recently Evanse *et al.*[14] performed molecular-dynamics studies of the deposition dynamics of individual atoms. In their simulations at a substrate temperature of 80 K the deposited metallic atom always settles into the hollow site of the substrate onto which it impinges. In such conditions one can obtain an atomically sharp interface between the metal and the substrate and a continuous film without an island structure due to the statistical nature of the atom distribution.[5,6,22,25,35]

As far as we know, a preliminary investigation of the growth morphology of the Ag/InAs(110) system was performed only in Ref. 7. Therefore to understand the large

TABLE I. Fitting parameters for the In 4d and As 3d core-level spectra of a clean InAs(110) surface taken with 101-eV photons. All energies are in eV.

	In 4d, LT	In 4d, RT	As 3d, RT
Spin-orbit splitting	0.87	0.87	0.69
Branching ratio	1.23	1.33	1.5
Gaussian width	0.3	0.43	0.45
Lorentzian width	0.25	0.25	0.17
BE shift of s	0.29	0.29	−0.36

disagreement between the electronic structures of Ag/InAs(110) systems formed at LT and at RT, we paid special attention to studying the differences in the growth morphologies at these two temperatures.

From the analysis of the evolution versus Ag coverage up to a few monolayers, of the surface (*s*), bulk (*b*), and interfacial (*i*) components of the core-level spectra as well as the comparison with the development of the valence-band (VB) spectra, we confirm the growth morphology previously inferred from low-energy electron diffraction (LEED) observations and Auger electron spectroscopy (AES) measurements.[7] Basically, the growth is laminar at LT, while it follows a VW mode at RT, with indications of some interactions between Ag and In atoms at both temperatures. Indeed a similar behavior has already been observed on other III-V substrates[1-5,35]

Let us pay attention to some core-level data. In Figs. 1(a) and 1(b). We show representative In 4*d* core-level spectra taken at RT and LT for Ag/InAs(110). The curves were background subtracted and normalized. The In 4*d* spectra of the clean surface could be decomposed into two components (*b* and *s*). Both at RT and LT the positions of In 4*d* *s* components are shifted by ≈0.29 eV to higher binding energy (BE) relative to the bulk ones. However, after silver deposition a new component (*i*) appears that is shifted by ≈0.5 eV to lower BE relative to the bulk one at LT as well as RT. At LT with increasing coverages the *i* component grows in relative intensity

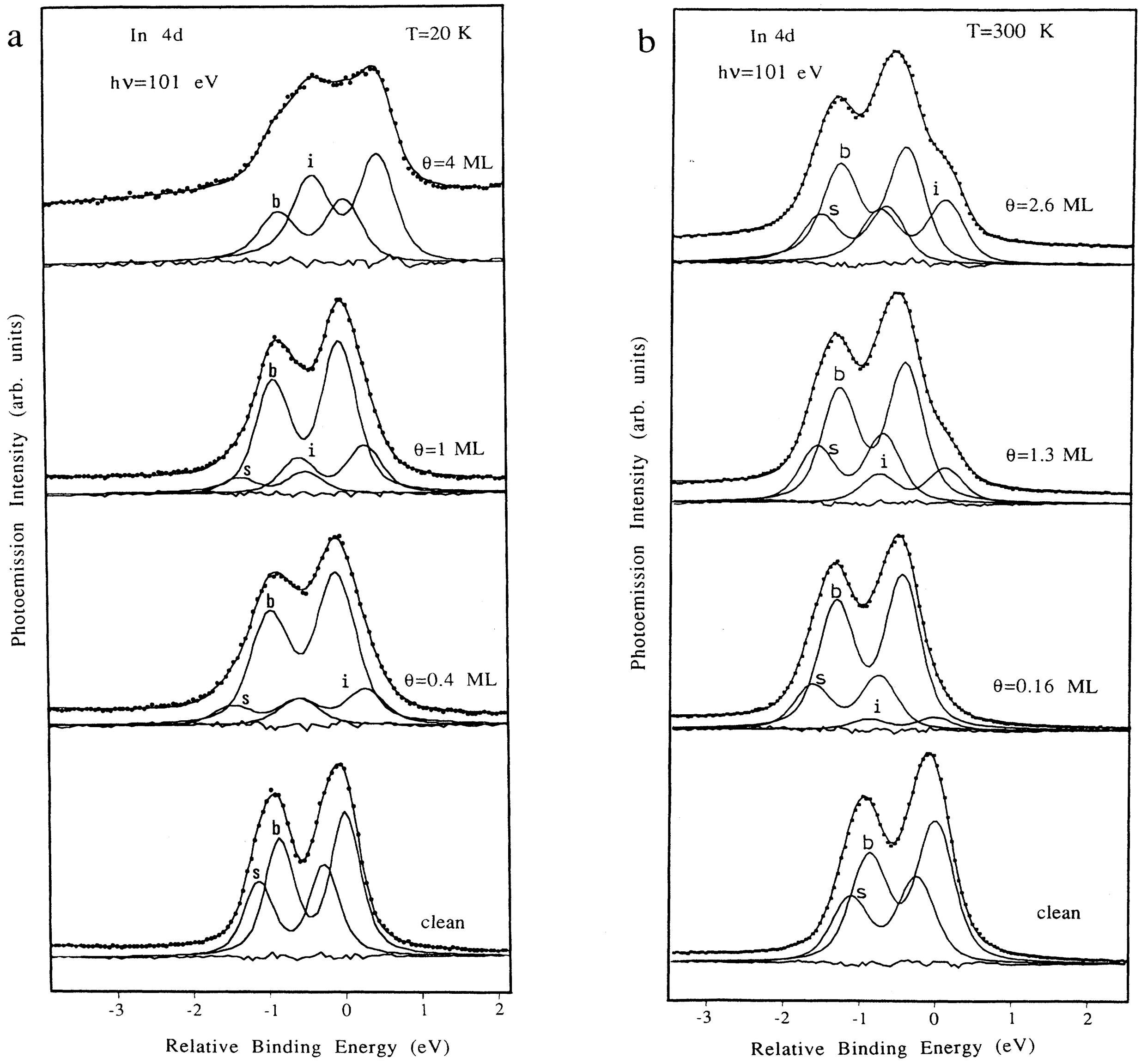


FIG. 1. (a) In 4*d* core-level spectra taken at $h\nu = 101$ eV of Ag/*n*-type InAs(110) at selected silver coverages, LT. Surface (*s*) and bulk (*b*) components from substrate and an "interface" component (*i*) due to the interaction at the interface are shown as well as the residuals of the fit. (b) Same as (a) for *p*-type InAs(110) at RT. (c) Same as (a) for As 3*d* core-level, *p*-type InAs(110), RT.

while the s component diminishes and disappears beyond about $\theta \approx 1$ ML.

Probably at this temperature the deposited Ag atoms just give some charge to the dangling bonds of the In atoms. The resulting charge in the dangling bonds becomes larger as compared to that of the bulk bonds. Therefore the s component is gradually transferred with coverage into the i component; the position of which is shifted to lower BE relative to the position of the b component. At $\theta \approx 1$ ML the dangling bonds are saturated and the s component is completely transformed into the i one.

The fact that the intensity of the i component at 4 ML [topmost spectrum in Fig. 1(a)] is relatively high as compared to the b component leads us to the conclusion that the homogeneity of the Ag film is very high: the interfacial atoms are placed at a sharp interface below the continuous silver film and on the top of the substrate: the b component is thus strongly screened. In fact, upon further Ag deposition at this temperature the b component completely disappears and one can observe only the i component with a very small signal.

In Fig. 1(c) we show representative As $3d$ core-level spectra taken at RT. The s component in the clean InAs As CL's is shifted by ≈ 0.36 eV to lower BE. We did not carry out systematic measurements of the As CL's spectra at LT. This allowed us to keep the surface uncontaminated at LT. However, we have taken a few of them at LT from clean surfaces and covered by Ag surfaces. First of all, we did not observe any i components as a result of Ag deposition neither at LT nor at RT. Thus we can eventually draw two conclusions. First, most probably the Ag atoms deposited onto the InAs(110) surface at RT or LT do not interact with As atoms. Second, one

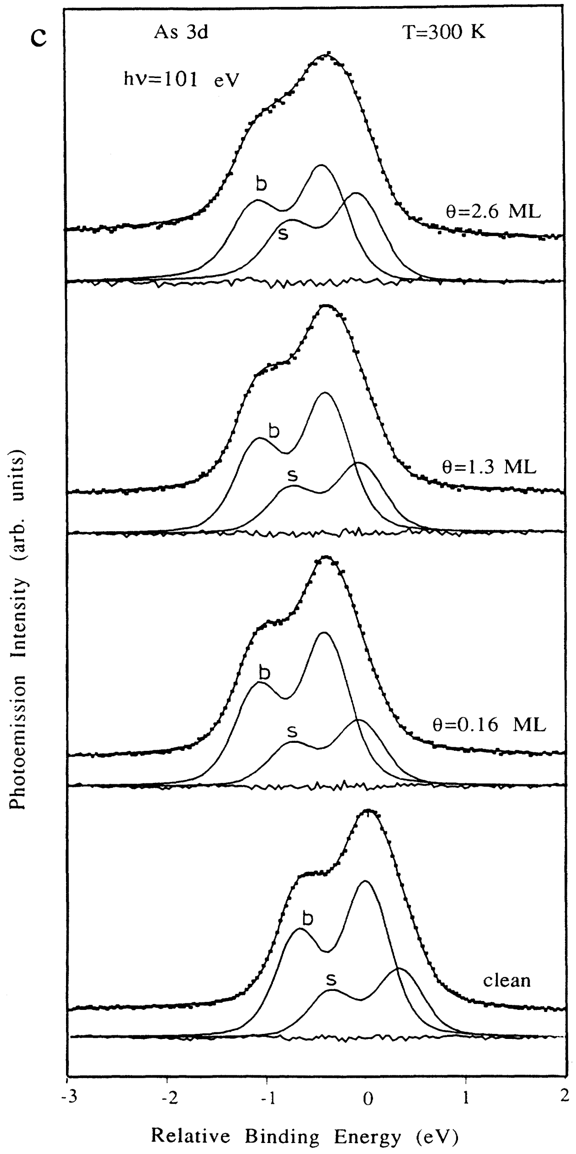


FIG. 1. (*Continued*).

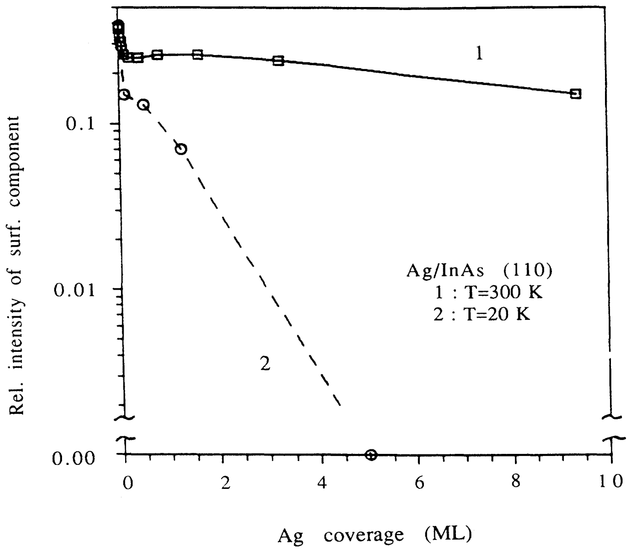


FIG. 2. Variations of the ratio I_s/I_t as a function of Ag coverage at LT (open circles) and RT (open squares). I_s is the surface component intensity and I_t is the total intensity of the In 4*d* core level.

can imagine that some charge is transferred from the As dangling bonds to the In dangling bonds (i.e., as result of derelaxation) or to the Ag atoms, but in this case the *i* component position coincides with the As 3*d* bulk component position. So from the In 4*d* and As 3*d* CL spectra taken at RT and LT from clean InAs(110) and after Ag deposition we can conclude, that probably only a weak interaction arises between the Ag atoms and the In 4*d* dangling bonds. And almost probably the Ag atoms are completely unreactive to the As atoms.

Now let us discuss the growth modes. From the analysis of the evolution of the *s*, *b*, and *i* components of the CL spectra shown in Figs. 1(a)–1(c) we conclude that the growth is laminar at LT and follows a VW mode at RT. The relative intensities I_s/I_t of the In 4*d* *s* components I_s as a function of θ, taken at LT (open circles) and RT (open squares) are shown in Fig. 2. (I_t is the total intensity of the In 4*d* core level.) The persistence of the *s* component in the In 4*d* and As 3*d* core levels up to high Ag coverages ($\theta \gg 1$) at RT is mainly the result of the VW growth mode at this temperature. The same conclusion could be reached from the results shown in Figs. 3(a) and 3(b), which display normal emission VB spectra at RT for the clean InAs(110) surface (a) and after deposition of 1 ML Ag (b). The intensity of the curves are nor-

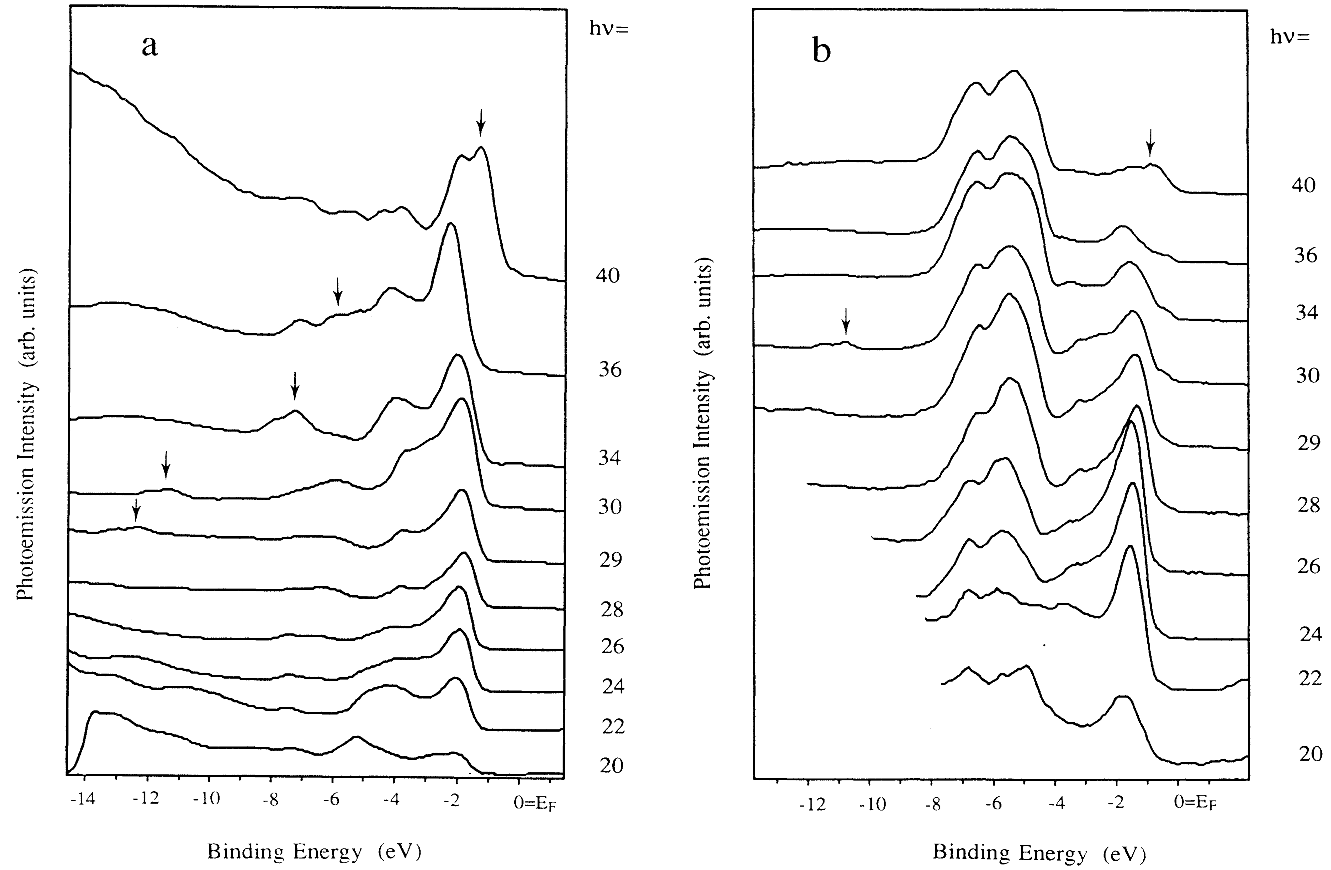


FIG. 3. Normal emission EDC's taken at different photon energies for (a) a clean InAs(110) surface and (b) after deposition of 1 ML Ag at RT. Binding energies are related to the E_F. ↓ denotes the As 3*d* peak of secondary order.

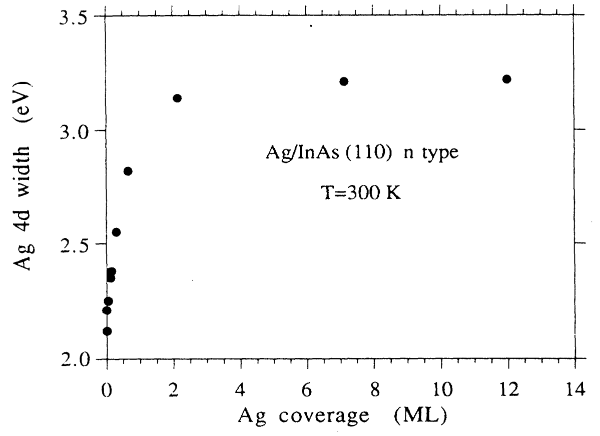


FIG. 4. Width of Ag 4d peaks from spectra taken at $h\nu=40$ eV as a function of coverage.

malized to observe the dispersion of the VB peaks. The main features of each energy-distribution curve (EDC) at a given photon energy are nearly the same for the two (clean and Ag covered) surfaces. The original VB peaks from the clean surface (a word of caution: coming closer to E_F with increasing photon energy is the As peak of second order) are very strong for both series of EDC's especially the sharp nondispersive peak at ≈ -2 eV (clean surface) attributed to a SS. It means that after deposition of 1 ML of Ag onto the InAs(110) surface the main part of the substrate remains clean and the island-growth mode takes place.

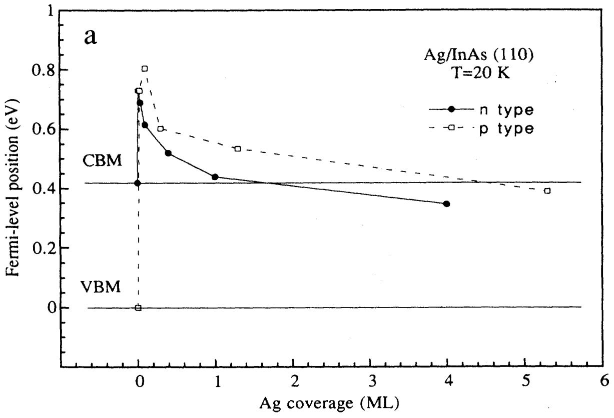
In Fig. 4 we show the width of the Ag 4d peak as a function of Ag deposition at RT. This evolution testifies that metallicity (full metallic bandwidth) is achieved between about 1 and 2 ML. This is further confirmed by a closer look at the change in shape of As 4d peaks and at the E_F region. The same conclusion could be made from Fig. 4(d), which shows the width of this Ag 4d peak as a function of Ag deposition.

The LT results suggest that at ≈ 20 K the Ag film growth is laminar. The LEED data[7] further support this conclusion. During deposition of the metal at LT a homogeneous background appears in the LEED patterns at very small values of θ; at around $\theta \approx 2-3$ ML all the substrate diffraction spots fade and only a uniform background is visible. An island mechanism for the Ag film growth at RT is confined by the LEED observations[7] as well: during Ag deposition at RT the substrate diffraction spots are still visible at 20 ML. The same growth mechanisms were also inferred from the comparison of the AES curves for both RT and LT depositions.[7] Moreover, in our previous low-electron energy-loss spectroscopy studies[6] we noticed that the surface excitons (In 4$d$$\rightarrow$In dangling-bond transitions) rapidly vanished (at $\theta \approx 1$ ML) upon LT Ag deposition onto the InAs(110) surface, however, they persisted up to 6 ML upon RT deposition.

V. ELECTRONIC STRUCTURE

Band-bending changes versus silver coverage were evaluated from the parallel shifts of the b components of the In 4d and As 3d core levels. An initial BB due to possible cleavage imperfections might have been a problem. As a matter of fact van Laar, Huijser, and Van Rosy[36] have shown that for InAs(110) the step-induced SS lay above the CBM however at a position lower than the bottom of the empty SS. At the edge of a step each metal atom has two equivalent dangling bonds. These induced states should be filled to about 20%. This means that we can expect E_F stabilization by steps for both n- and p-type InAs(110) if such states exist above the CBM (downwards initial BB). We have retained, however, only high-quality cleavages with flat bands: the measured differences between the b components in the core-level spectra of our n- and p-type samples correspond to the InAs band-gap values (for both RT and LT measurements) in a reproducible manner. Since we chose highly doped (nearly degenerate) n- and p-type samples, the initial E_F positions are, respectively, close to the CBM and VBM and the shift of the core-level bulk components throughout the experiments corresponds to the displacement of the position of the E_F at the surface with respect to the bulk.

Figures 5(a) and 5(b) present the E_F positions at the surface as a function of Ag deposition on the InAs(110)



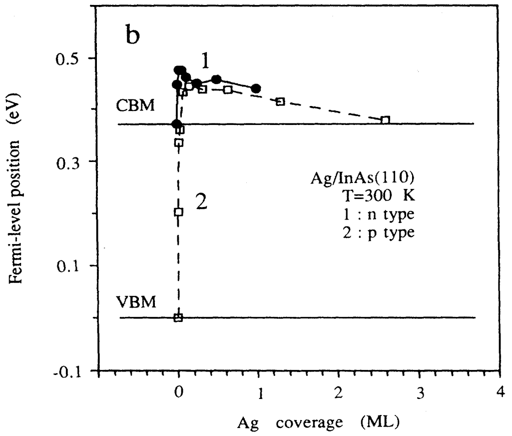


FIG. 5. (a) Position of E_F at the InAs(110) surface as a function of Ag coverage at LT for N-type (open) and p-type (closed) symbols. The E_F positions at the clean surfaces correspond to the VBM and the CBM of bulk for n- and p-type samples, respectively. (b) Same as (a) for RT.

cleaved surfaces at (a) ≈ 20 K and (b) ≈ 300 K. As shown before, right after the cleavage, flat-band conditions are obtained and the surface E_F levels are close to the CBM for n-type InAs or to the VBM for p-type InAs, respectively, as typical for all $A^{\mathrm{III}}\mathrm{B}^{V}$ compounds (except for GaP).[36] At LT during Ag deposition the position of E_F at the surface of n- and p-type InAs depends on the coverage θ in a dramatic fashion: it passes through a sharp and extremely high maximum equal to $E_C+(0.3-0.4)$ eV at $\theta \approx 0.01-0.1$ ML (E_C—energy of the CBM). This giant (≈ 0.8 eV on p-type) movement of E_F well into the conduction band (CB) thus creates an extremely strong 2D electron channel. Upon RT Ag deposition, E_F reaches lower maxima about $E_C+0.1$ eV for both n- and p-type samples almost at the same coverages.

It looks as if E_F is pinned by surface states of two types: the first ones are formed in the process of Ag deposition on the substrate cooled down to ≈ 20 K at very low coverages. The second ones correspond to rather high coverages for the two temperatures studied.

Now let us evaluate how much this result could be affected by synchrotron radiation illumination. To set aside any possible SPV effect even on this small gap semiconductor we have chosen highly doped, nearly degenerated, n- and p-type samples. In addition we have carried out Kelvin probe measurements, both under illumination and in the dark, at $T \approx 20$ K and $T \approx 300$ K. This method[29–32] does not use photons at all. First of all we performed measurements of the contact potential difference (CPD) of cleaved n-type InAs(110) surface as a function of Ag coverage at RT. After each additional deposition we have measured the CPD in the dark, under strong illumination and in the dark again. Figure 6 displays these values. We did not find any difference between the results obtained in the dark and under illumination. Furthermore, this result is in good agreement with that shown in Fig. 5(b). Indeed we assume that these CPD changes are the results of BB only and do not involve changes of the ionization energy (which is a common assumption). We notice also that due to nearly identical values of the Ag, As as well as In electronegativities,[30] the surface dipole induced by $\approx 0.01-0.1$ ML Ag is expected to be insignificant. In addition we carried out a few CPD measurements at LT and did not observe any SPV effect. To be even more certain we also carried out a few measurements with different slit settings. Decreasing the photon flux more than ten times does not influence the BB again. Thus we can conclude that our BB results are not affected at all by the synchrotron radiation illumination.

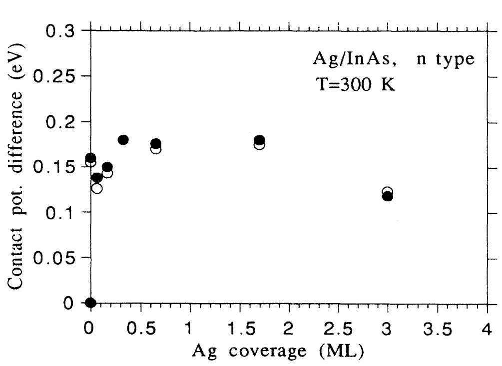


FIG. 6. Contact potential difference of a cleaved InAs(110) surface as a function of Ag deposition at RT. Closed symbols, results of measurements in the dark; open ones under illumination.

Still remains a question: one might expect the possibility of observing some emission from the 2D electron gas after E_F is moved well above the CBM. Yet, it is well known that the density of states in the band, ρ, is proportional to $m_{\mathrm{ef}}^{3/2}$, where m_{ef} is the effective mass of the electron. However because of the very small value of m_{ef}, ρ near the CBM in InAs is very low and one should not expect strong emission from this energy region. Nevertheless in Fig. 7(a) we show EDC's from the clean InAs(110) surface (it is shifted to higher BE from its original position to adjust the BB, that took place after Ag deposition) and in Fig. 7(b) after deposition 1 ML Ag at RT. The spectra are background subtracted and normalized to the same height of the surface peaks. The density of states near E_F in (b) can be interpreted as due to electron emission from the 2D gas discussed above. However we could assume also different explanations. (i) We detect the beginning of metallic step formation as a result of the creation of the 3D Ag island; (ii) this emission could come from SS that are moved from a high to a lower energy position in the conduction band as a result possibly of the derelaxation of the InAs(110) surface upon Ag deposition. Whatever the true explanation is this is the first direct observation of electron emission from states close to and above the CBM at the surface.

Now let us envisage the possible reasons which cause E_F to move well above the CBM. As we have shown earlier, at LT surface diffusion is essentially suppressed. Hence a uniform coverage with a statistical distribution of adatoms on the surface arises while the interaction between Ag atoms and the substrate is weak. Therefore at low coverages and LT there most probably exists donor-

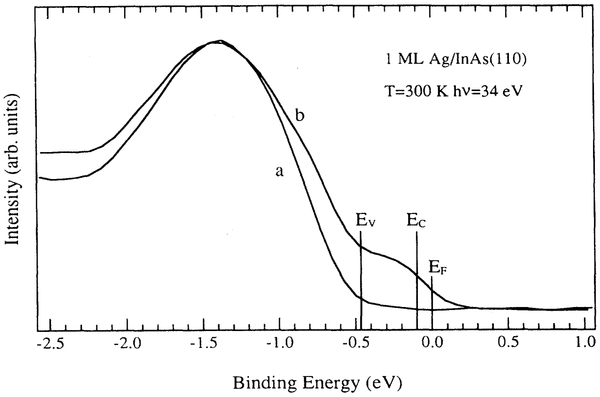


FIG. 7. EDC's taken near the VBM at RT: (1) from the clean InAs(110) surface (shifted to higher BE from the original position to adjust BB, that took place after Ag deposition) and (2) after deposition 1 ML Ag at RT. The spectra are background subtracted, and normalized to the same height of the surface peaks.

like AIS.[15] Let us assume that these AIS are situated at the energy $\approx E_C+(0.3-0.4)$ eV; then E_F can be pinned by these SS in the conduction band. This leads to the formation of a 2D electron channel at the InAs surface already at $\theta \approx 0.01-0.1$ ML for both types of semiconductor. At higher coverages one observes the onset of metallization (see above) for both temperatures and Ag clusters can produce another type of SS, typically MIGS (Refs. 8–11) near the CBM. This proposal is in a good agreement with the theoretical calculations of the MIGS for InAs.[37–39]

At RT and for small coverages there may be also two possibilities. First, before the metallization onset more reactive (as compared to LT) individual Ag atoms produce, for example, defect SS, placed near $E_C+0.1$ eV. Second, the situation is the same as at LT, however metallicity appears at lower coverages. Similar suggestions that adsorbed metallic atoms could create donor-type SS were proposed before by Mönch[15] as well as Flores, Batra, and Scheffler together with their respective co-workers[16–18] to explain the behavior of, e.g., alkali metal on GaAs. But in that case the E_F was pinned inside the gap.

VI. CONCLUSIONS

To summarize, by evaporating a very small amount of Ag onto well-cleaved InAs(110) surfaces a giant downwards BB occurs both on *p*- and *n*-type substrates at LT. This creates a strong 2D electron channel at these surfaces, which confers a very unique character to this metal/$A^{\mathrm{III}}B^{\mathrm{V}}$ semiconductor system.

Note added: It is interesting to mention that similar results have been also obtained recently for the Ag/InSb(110) interface by Aristov *et al.*[40]

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