Low-temperature formation of metal/molecular-beam epitaxy-GaAs(100) interfaces: Approaching ideal chemical and electronic limits

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We report soft x-ray photoemission studies of metal/molecular-beam epitaxy (MBE)-GaAs(100) interfaces formed at low temperature. Our results indicate that rectifying barrier heights are proportional to the metal work function in accordance with Schottky's original description of metal–semiconductor contacts. These results confirm the predictions of a self-consistent model of metal–semiconductor interfaces, and suggest that metal-induced gap states and native defect mechanisms are not major factors in determining the Fermi level energy at "ideal" interfaces. We attribute deviations from the ideal Schottky limit behavior observed for interfaces formed at room temperature to metallization-induced atomic relaxations (rather than electronic relaxations) occurring at metal–semiconductor contacts. We present a useful methodology for analyzing electronic properties at metal–semiconductor interfaces. The pronounced differences in barrier height formation between MBE vs melt-grown GaAs can evidence the role of deep states in controlling Schottky barriers at metal/melt-grown GaAs.

I. INTRODUCTION

Fifty years ago, W. Schottky introduced a model of metal–semiconductor junctions predicting that the rectifying barrier height is equal to the difference between the work function of the metal and the electron affinity of the semiconductor.[1] However, the lack of experimental evidence to support this model (barrier heights were found to be essentially metal independent) has motivated the development of several models aimed at explaining the origin and universality of Fermi level "pinning."[2,3] This widely accepted perception has been challenged in recent years. New experimental developments have increased our ability to grow high-quality materials (i.e., epitaxial growth methods)[4] and to determine some of the microscopic details of the chemical and electronic changes associated with the formation of solid interfaces.[5–8] Overall, these investigations have challenged the pinning concept as a general characteristic of rectifying contacts for covalently bonded semiconductors.[9,10] Rectifying barrier heights at most of the studied metal/III–V compound semiconductor interfaces have recently been found to be metal-dependent and distributed over a range of values of the order of the semiconductor band gap.[11–17] In general, new experimental observations indicate that extrinsic phenomena strongly influence the interface electronic properties, i.e., chemical reaction and interdiffusion take place concurrently which promote formation of localized charge states and changes in interface electronic potentials.[18–22] The complexity in the chemistry and physics of metal–semiconductor interfaces has prevented the full evaluation of the theoretical models. Recent studies have inspected the effect of temperature on the properties of metal–semiconductor interfaces.[23–25] These experiments have shown that metal overlayers are more uniform and interfacial chemical reactions are reduced at low temperature, usually below 100 K. Consequently, low-temperature studies represent a unique opportunity to test theoretical models and to establish ideal limit behavior of metal–semiconductor interfaces.

In this paper we report soft x-ray photoemission spectroscopic studies of metal/molecular beam epitaxy grown (MBE-) GaAs(100) junctions formed at low temperature. We present measurements of Fermi level movements (band bending) as a function of metal coverage, their correlation with the onset of metallic character of the overlayer, and the dependence of the interface electronic properties on specific metal–semiconductor reactivity. These results indicate that the rectifying barrier at ideal interfaces is indeed proportional to the metal work function in accordance with Schottky's original description and with a recent self-consistent model of metal–semiconductor interfaces.[26] We compare our results with those recently reported for melt-grown GaAs(110) interfaces at low temperature.[23–25] This comparison highlights the role of bulk crystal quality in controlling the Schottky barrier formation of metal/melt-grown GaAs.

II. EXPERIMENT

Soft x-ray photoemission spectroscopy (SXPS) experiments were performed at the 1-GeV ring of the SRC, University of Wisconsin–Madison. The sample temperature was maintained below 100 K (LT) during evaporation and measurements. We measured bulk (surface) sensitive spectra of As 3*d* and Ga 3*d* core levels using $h\nu = 55$–60 eV (100 eV) and 35–40 eV (80 eV), respectively. These energy sets produce photoelectrons with nearly identical escape length,

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~ 15 Å (5Å), for As and Ga at kinetic energies of about 9–14 eV (54 eV). Thus, the core-level SXPS spectra show similar depth resolution for both elements. We measure Fermi level (E_f) movements with metal deposition from shifts in Ga 3*d* and As 3*d* core level positions. The bulk/surface sensitive spectroscopy allows us to distinguish core level shifts due to energy band movements from contributions due to chemical shifts.[10]

The As-coated MBE specimens have an unstrained, epitaxial overlayer, Ohmic contact layer structure consisting of a 7500-Å-thick GaAs ($n = 5\times10^{15}$–5×10^{16} Si/cm^3) grown over a 2000-Å layer of MBE GaAs ($n = 2\times10^{18}$ Si/cm^3) on top of an n + GaAs(100) substrate. Clean ordered MBE-grown GaAs(100) surfaces were obtained by thermal desorption of the As protective cap in ultra high vacuum (UHV).[22] Metals were evaporated from outgassed W-baskets on the clean surfaces held at LT and film thicknesses were monitored by means of a quartz crystal oscillator positioned next to the specimen surface. Monochromator scan energies, signal acquisition, rate of heating, and mass spectrometer were controlled by a microcomputer.

III. RESULTS

A. Fermi level movements at low-temperature metal/MBE-GaAs(100) junctions

Figure 1 shows Fermi level movements with respect to valence-band (VB) edge E_v as a function of Ag, Al, Au, Cu, In, and Yb coverages on n-type MBE-grown GaAs(100). The figure indicates a common trend in E_f movements with metal deposition for the interfaces investigated. Metal deposition up to a few Å thickness causes a small upward shift of E_f. Subsequent metal deposition causes large E_f movements at particular metal thicknesses. The final measured E_f positions depend strongly on the deposited metal, and they range over much of the semiconductor band gap. Indeed, Fig. 1 indicates an E_f range which extends over 0.93 eV, from E_v + 0.37 eV to E_v + 1.30 eV. These values expand the observed 0.7 eV range for similar metal/MBE-GaAs(100) interfaces formed at room temperature (RT).[15] Our results are in striking contrast with those reported for low-temperature metal/melt-grown GaAs(110) interfaces.[23–25] First, the low coverage region (metal thickness up to a few Å) shows E_f movements for both GaAs materials, but in opposite directions. Figure 1 indicates that LT n-type MBE-GaAs(100) surfaces consistently shown E_f upward shifts from the initial E_f position at ~E_v + 1.3 eV, whereas LT n-type melt-grown GaAs(110) surfaces consistently show E_f downward shifts from the initial E_f position of the cleaved surface at E_v + (1.4 ± 0.05) eV.[23–25] Second, for large metal coverages, melt-grown GaAs(110) surfaces show final E_f values essentially independent of the metal and temperature of interface formation,[23–25] on the other hand, our results indicate a temperature-dependent wide final E_f range for MBE-GaAs(100). Some similarities in the kinetics of interface formation are found for both GaAs materials, i.e., the rapid E_f movements which occur at several Å metal coverages.[23–25]

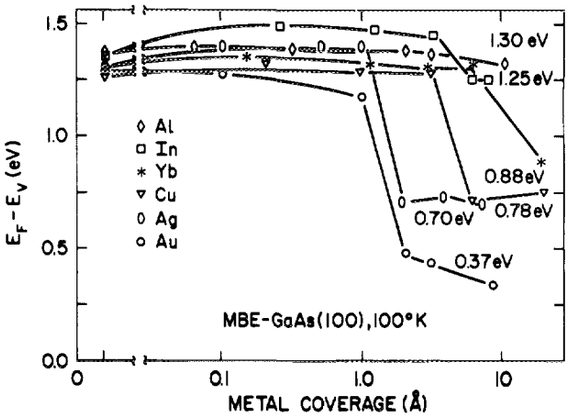

FIG. 1. E_f movements as a function of metal coverage for Ag, Al, Au, Cu, In, and Yb deposited on n-type MBE-GaAs(100) at 100 K.

B. Band bending and overlayer metallic character

The onset of metallic character in the overlayers was measured from changes in metal adsorbate photoemission features with increasing metal thicknesses. Figure 2 shows valence-band photoemission spectra of a clean ordered unpinned n-type MBE-GaAs(100) surface as a function of increasing Cu thicknesses. The arrows indicate the evolution of specific Cu photoemission features with increasing metal deposition. The VB spectrum of the 0.2 Å Cu coverage

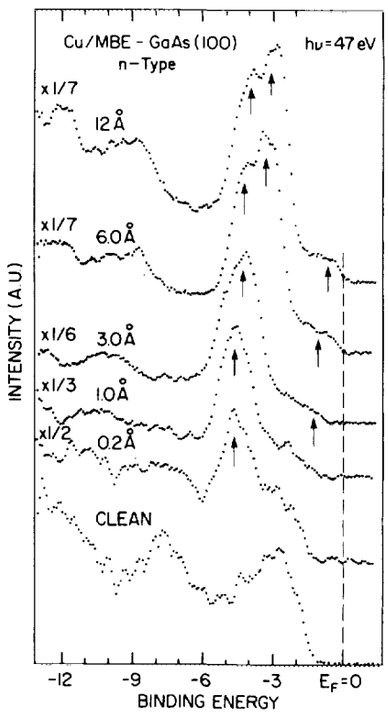

FIG. 2. Valence-band photoemission spectra of MBE-GaAs(100) as a function of Cu coverage.

shows a new peak at binding energy (BE) ~ -4.5 eV, which corresponds to Cu $3d$ levels.[27] This submonolayer VB spectra show that only a small perturbation of the GaAs substrate occurs upon metal deposition: the VB edge shows no shift and the main features of the spectral shape of the GaAs substrate are unchanged. Substantial change in the VB spectrum occurs between 3 and 6 Å metal coverages. The 6 Å coverage VB spectrum shows a broadening of both the Cu $3d$ peak and the $4s$ levels, which extends to the E_f of the system. The Cu $3d$ peak evolves from a single peak at low coverage to the doublet structure characteristic of metallic Cu d bands at higher coverages. These changes in VB spectral features with increasing metal thickness are characteristic of the onset of metallic behavior.[25,28,29] These changes were observed in all the metal/GaAs VB spectra at particular metal coverages. Variations from metal to metal also include the d band width (when present) and band position relative to E_f. The VB edge position of the 6 Å Cu/MBE-GaAs(100) interface lies within 0.1 eV from the E_f of the system. This bulk E_f was measured from a 200 Å fresh Au film deposited under UHV conditions on an electrically grounded Ta substrate. For the 12 Å Cu/MBE-GaAs(100) interface, the band edge lies within 0.02 eV of the bulk E_f. These differences between the bulk E_f and the interface E_f of thin metal films are due to final-state charging effects[25,29] and are in fact an artifact of the photoemission measurement. The onset of the metallic character observed in the 6 Å Cu VB spectrum correlates with the fast change in E_f measured from bulk-sensitive rigid Ga $3d$ and As $3d$ core level shifts. This correlation was observed for all the interfaces studied.

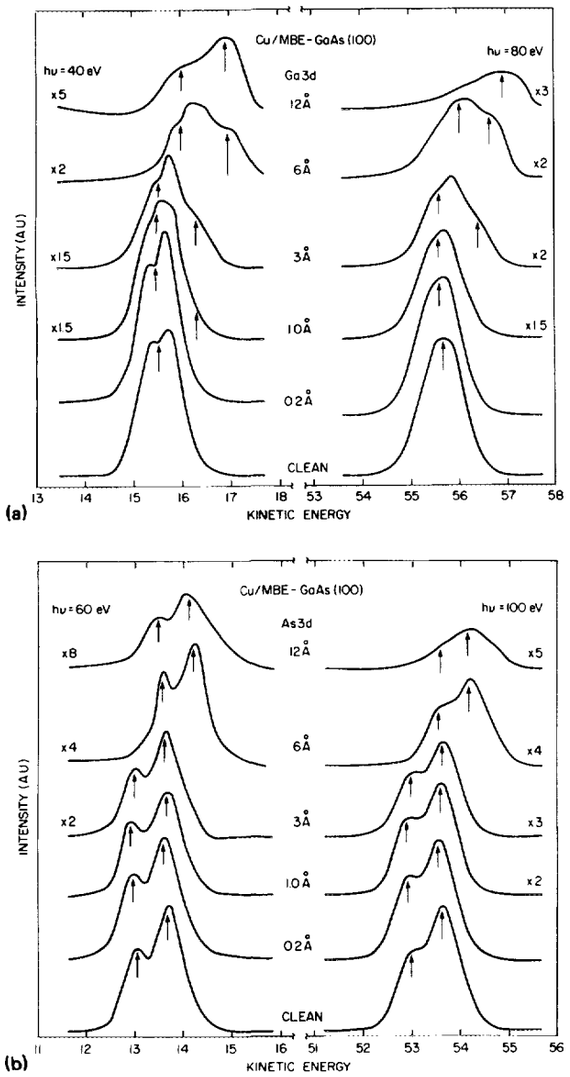

FIG. 3. Core level photoemission spectra of MBE-GaAs(100) as a function of Cu coverage. Bulk and surface sensitive features for (a) Ga $3d$ and (b) As $3d$ core levels. The Ga $3d$ and As $3d$ core level spectra exhibit rigid shifts at 6 Å Cu coverage due to band bending.

C. Core level spectra and metal–semiconductor interactions

Core level photoemission spectra were used to measure band bending and detect chemical interactions which occur at the semiconductor surface upon metal deposition. Figure 3(a)–3(b) show Ga $3d$ and As $3d$ core level spectra and illustrate the changes produced on n type MBE-GaAs(100) surfaces by increasing Cu deposition. With initial metal deposition, both Ga $3d$ and As $3d$ peaks shift to lower kinetic energy. This shift of the core levels with submonolayer metal deposition was observed in almost every metal/GaAs system. The magnitude of the shift shows small variations from system to system, between 50 to 150 meV, and is observed in both the bulk- and surface-sensitive spectra. These measurements suggest that the core level shifts correspond to an E_f movement toward the conduction band from the initial E_f position of ~ 0.20 eV below the conduction band minimum as shown in Fig. 1. At 6 Å coverage a large shift is observed for both Ga $3d$ and As $3d$ spectra. This shift, measured from the bulk sensitive Ga $3d$ (40 eV) and As $3d$ (60 eV) spectra, corresponds to upward band bending of ~ 0.47 eV from the initial E_f position at $E_v + 1.25$ eV to $E_c + 0.78$ eV. The evolving shoulder observed on the high kinetic energy side of the 3 Å Ga $3d$ surface- and bulk-sensitive spectra indicates a small fraction of dissociated Ga. This dissociated feature dominates the Ga $3d$ spectral shape for increasing metal coverages due to the attenuation of the substrate contribution to the total spectral intensity. The As $3d$ spectra show no new features with increasing Cu deposition.

Figure 3 indicates that chemical interactions between the MBE-GaAs substrate and the deposited metal were not totally suppressed, but only reduced, at the low-temperature achieved in our experiments. In most cases, there was little indication of reaction or interdiffusion. An exception was the Yb/MBE-GaAs(100) experiment. Here, we observed the formation of broad spectral features for both Ga $3d$ and As $3d$ core level spectra. This spectral broadening indicates the presence of a large amount of reacted components at the interface. These reacted components dominate the emission with increasing Yb deposition. This fact made the measurement of the E_f position for Yb overlayers extremely difficult. We report here the E_f value as determined from each intensity maximum of the broadened core level spectra. This E_f

value is close to that obtained for RT Yb interfaces to MBE-GaAs(100), although evidence for a Fermi level position closer to the conduction band edge may be masked by the reacted component spectra. The extensive reaction observed during the Yb experiment may be due to the Yb high reactivity and large atomic volume, which can easily disrupt the GaAs surface. Other possibilities for the observed extensive reaction are deposition rate, of about 0.5 Å/s, and the LT conditions achieved (100 K), which may not be low enough to inhibit highly reactive metals from generating extensive substrate disruption.[19]

D. Schottky barrier heights at metal/MBE-GaAs(100) junctions

Figure 4 shows Schottky barrier heights (SBH) as a function of metal work function for LT metal/MBE-GaAs(100) interfaces. The values of the rectifying barriers were obtained by subtracting the measured E_f-E_v energies from the GaAs band gap (1.51eV at 100 K).[30] Figure 4 indicates that the range of SBH's extends to ~1 eV for these metal–semiconductor junctions. The inset in the upper left corner indicates the energy band diagram for ideal Schottky behavior, and corresponds to the diagonal line shown. This line was calculated using the reported value of the electron affinity of the (110) face of GaAs equal to 4.07 eV.[31] We expect only minor differences between this value and the electron affinities of the distinct reconstructions of the (100) face of GaAs.[32]

IV. DISCUSSION

This section is organized as follows: first, we discuss the implication of our results on the different models of rectifying contacts and propose a methodology for analyzing electronic properties at metal–semiconductor contacts. Then we compare interface behavior of both MBE- and melt-grown GaAs.

The results shown in Fig. 4 clearly indicate that SBH's at low-temperature metal/MBE-GaAs(100) interfaces range over the semiconductor band gap and closely follow the predictions of the classical Schottky model, that is, the rectifying barrier height scales with the difference between semiconductor and metal work function. Consequently, these results strongly suggest that models predicting pinning, via metal-induced gap states[33] (electronic relaxations) or native defect mechanisms,[34,35] are of little relevance in determining the position of the interface Fermi level at these ideal metal–semiconductor interfaces. However, a self-consistent model which does not explicitly consider atomic rearrangements at the metal–semiconductor interface relative to the vacuum surfaces[26] has provided a microscopic derivation of Schottky's phenomenological description of metal–semiconductor junctions. In the absence of extrinsic localized charge,[26] the main prediction of this model is described by the Schottky limit line shown in Fig. 4. The close agreement between model predictions and experimental results indicates that *the Schottky boundary conditions are indeed appropriate to describe ideal contacts.* These experimental and theoretical results imply that the insensitivity of the rectifying barrier height to the metal work function, i.e., the SBH's reduced range and pinning observed at real contacts, has its origin in atomic (rather than electronic) relaxations at the interface. Therefore, the Schottky boundary conditions can

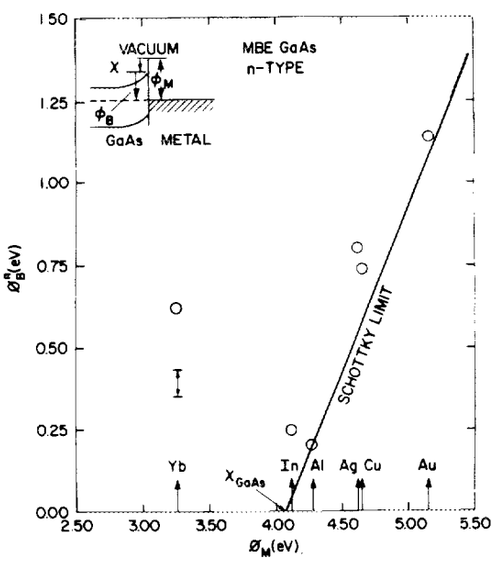

FIG. 4. Experimental Schottky barrier heights for Ag, Al, Au, Cu, In, and Yb contacts to MBE-grown *n*-type GaAs(100) at LT. The inset in the upper left corner represents ideal Schottky behavior, and corresponds to the diagonal line shown. Here we use the electron affinity for GaAs(110) (4.07 eV).

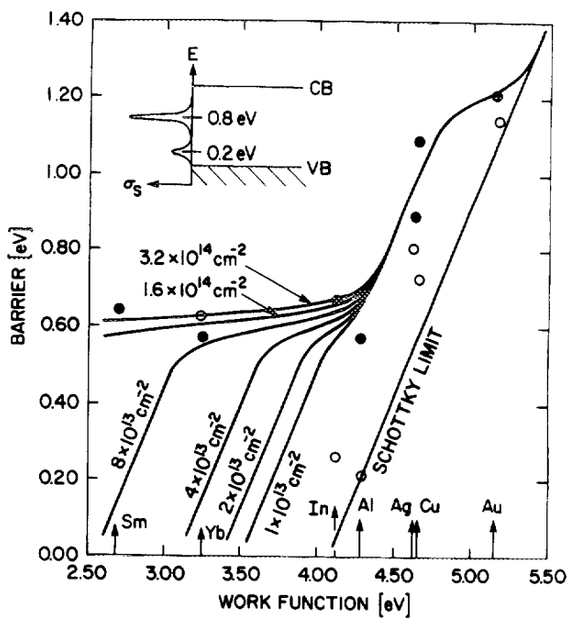

FIG. 5. Experimental Schottky barrier heights for several metals at both LT (open dots) and RT (dots) interfaces to *n*-type MBE-GaAs(100). Model calculation of SBH's including interface acceptor states with energies at 0.8 and 0.2 eV. The interface state energy positions are illustrated in the upper left corner inset.

serve as the basis for the general description of metal/III-V semiconductor junctions.

Extensive atomic rearrangements, i.e., those which occur at metal–semiconductor interfaces formed at room temperature, account for deviations from the ideal Schottky behavior. Figure 5 illustrates the differences in SBH's between metal/MBE-GaAs(100) interfaces formed at LT (open circles) and RT (circles)[16] as a function of metal work function. These differences are due to metal–semiconductor interactions, which are responsible for interfacial atomic rearrangements leading to the formation of interface charge states and changes in solid–solid interface electronic potentials at the junction. Variations in surface electronic potentials with atomic rearrangements at vacuum-solid interfaces are well documented.[36] Using low-energy cathodoluminescence spectroscopy we have provided experimental evidence for the formation of discrete charge states at metal/GaAs interfaces, for some of their properties and their quantitative and qualitative correlations with particular metal, specific crystal face, and material quality.[6,22]

In order to perform theoretical calculations to explain deviations from the ideal Schottky behavior we must know the positions of the atoms at the real metal–semiconductor interface. Such information is, at present, unavailable. In the interim, we have adopted the following phenomenological approach to describe the consequences of the atomic rearrangements on the SBH: As a first step, we postulate that reaction-induced interface charge states are the main cause of deviation from the Schottky limit behavior.[26] Then, we can estimate the nature of the interface states (donors, acceptors, etc.), their energies and effective concentrations from the dependence of the measured SBH on the metal work function and the energies of the optical emission from reaction-induced interface states. The results of such calculations have been reported previously.[9] Figure 5 reproduces the calculated rectifying barrier heights, together with the experimental RT (dots) and LT (open dots) SBH's as a function of metal work function. Comparison of our data with the density-dependent curves shows that metallization of GaAs creates interface charged centers whose maximum total effective concentrations are in the low 10^{14} cm^{-2} range. These numerical results also indicate that the concentration of the interface acceptor state at ~ 0.8 eV controls the barrier heights for low work function metals. A refinement in the treatment of the interface charge states consists of considering delocalization effects at metal–semiconductor interfaces.[37]

The second step, yet to be accomplished, consists of modeling the atomic-rearrangement-induced change on metal work function and semiconductor electron affinity. The Effective Work Function (EWF) model of Freeouf and Woodall[38] directly addresses this issue. Within the EWF model the presence of excess As at the interface dominates the metal work function. A refinement of this model consists of varying the relative amounts of intermixed metal atoms, As, and Ga, for particular systems, thereby assessing their specific contribution to the work function. Measurements of changes in metal work function upon adsorption of minute amounts of As, Ga, and both on clean metal surfaces could provide a sufficient data set to model the main aspects of work function behavior.

The wide range of SBH's obtained at LT MBE-GaAs(100) surfaces emphasizes the previously reported differences in interface behavior between MBE-GaAs(100) and melt-grown GaAs(110) at room temperature.[10,15] Experiments involving low-temperature interface formation of metal/melt-grown GaAs(110) have demonstrated the correlation of E_f movements with the onset of metallic character.[25] However, no major differences were found between final E_f positions for both RT and LT interfaces.[23–25,32] Controversial interpretations include control of final pinning position by metal induced gap states (MIGS),[25] and delayed formation of defect levels attributed to delayed cluster formation.[24] However, our results strongly suggest that pinning behavior is a direct consequence of extrinsic phenomena. Several factors which can contribute to the narrow range of SBH's observed at UHV-cleaved, melt-grown GaAs(110) surfaces have either little or no influence on MBE-GaAs(100).[10,16] These factors include specific surface reactivity of the semiconductor surface,[10] excess As,[38] bulk traps,[10,15] nature of the interface states,[22] and material inhomogeneities.[10,39] The effect of temperature on these factors is poorly understood. There is clear evidence that surface reactivity is reduced at low temperature, although a quantitative account of this effect is yet to be achieved. On the other hand, the striking differences in interface behavior between MBE-[10,16] and melt-grown GaAs[23–25,35] at both LT and RT can be indicative of the role that deep levels (either created at the surface, segregated, or activated by some other mechanism) are playing in determining the pinning behavior observed at metal/melt-grown GaAs interfaces.

V. CONCLUSIONS

The wide predictable range of Fermi level control displayed by different metals on MBE-GaAs(100) surfaces at low-temperatures provides one of the strongest tests which can be applied to models of Schottky barrier formation. Our soft x-ray photoemission studies of a variety of metal/MBE-GaAs(100) interfaces formed at LT indicate that rectifying barrier heights scale with the work function of the deposited metal and follow closely the classical Schottky-like behavior. These results confirm the predictions of a self-consistent model of metal–semiconductor interfaces, and suggest that metal-induced gap states and native defect mechanisms are not major factors in determining the Fermi level energy at ideal interfaces. Deviations from the ideal Schottky limit behavior observed at interfaces formed at room temperature are caused by metallization-induced atomic relaxations occurring at metal–semiconductor contacts. We suggest a methodology for analyzing electronic properties at metal–semiconductor interfaces and propose that the presence of deep levels causes the pinning behavior observed at metal/melt-grown GaAs interfaces.

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