METAL-GaAs(110) INTERFACES FORMED AT LOW TEMPERATURE:
FROM ADSORBATE- TO METAL-INDUCED GAP STATES

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I. INTRODUCTION

After two decades of research on metal-semiconductor interfaces, the problem of the formation of Schottky barriers is still very much present (and controversial)\(^1\). The origin and nature of the interface states which pin the Fermi level (\(E_F\)) at metal-semiconductor interfaces remain uncertain. The difficulty in resolving this issue stems from the diversity of metal-semiconductor interfaces and from the complexity of their chemistry, morphology and atomic structure. Progress has been made in the understanding of the microscopic structure of some of these interfaces with low energy electron diffraction (LEED)\(^2,3\), ion channeling\(^4\), total energy minimization calculations\(^5,6\) and with the recent development of scanning tunneling microscopy\(^7\). Enough remains unknown, however, that interface structure, interdiffusion, defects or metallization still raise unanswered questions about the pinning process. In addition, Vitturo et al. have recently indicated that deep levels in the bulk of the materials used for most Schottky barrier formation studies, i.e. liquid-encapsulated Czochralski GaAs, might be responsible for the narrow range of \(E_F\) pinning in the gap, and that pinning occurs in a much wider range on (100) surfaces of substrates grown by molecular beam epitaxy\(^8\). This result adds another dimension to an already difficult and overly discussed subject.

From the point of view of electronic and atomic structures, the best understood semiconductor surface is GaAs(110)\(^2\). It has no intrinsic surface states in the gap, and this has led to extensive work on the formation of metal-GaAs(110) interfaces. These prototypical interfaces exhibit a wide range of structural and chemical behaviors. Some are abrupt (In, Ag)\(^9\) or interdiffused (Au)\(^10\), reacted (Mn, Ca, Ti)\(^11,12\) or chemically inert (In, Ag, Ga)\(^9,11\), quasi two-dimensional (Sb, Sn)\(^13–15\) or composed of three-dimensional clusters (Ag, In)\(^9\). Yet, the rate of band bending and the final pinning position of the Fermi level are quite

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comparable at all these interfaces. The simultaneity of various interface events such as reactions, metal clustering or atomic relaxation has so far obscured the identification of the dominant $E_F$ pinning mechanisms. With low metal coverage, during the initial stages of the formation of the barrier, the experimentalist deals with systems which are far removed from the ideal, and often atomically ordered, interface modeled by the theorist. It is indeed far too difficult at this time to do theory on these real interfaces.

One of the techniques used in the past few years to circumvent this difficulty is the formation of metal-semiconductor interfaces at low temperature (\textasciitilde 70-100 K)\textsuperscript{9,11,15-18}. It is expected, and verified in most cases, that interface reaction, interdiffusion and clustering are considerably inhibited at LT and that the complex interface is "simplified". Although the interface formed at LT is "frozen", and is therefore somewhat different from its RT counterpart, valuable information on the overall $E_F$ pinning process can be obtained. In particular, LT provides a more accessible step-by-step formation of interfaces and helps identify more readily the dominant pinning mechanism(s) for various coverage regimes.

During the past three years, we have investigated interfaces formed between LT GaAs(110) and Al\textsuperscript{9,19}, In\textsuperscript{9}, Ag\textsuperscript{9,17,20}, Au\textsuperscript{9,20}, Pd\textsuperscript{21} and Sn\textsuperscript{15}. A trend in band bending, different from the room temperature (RT) band bending, was observed at all these interfaces. This forced a reevaluation of the Schottky barrier formation problem in a way which tends to reduce the role of interface defects and emphasize the importance of adsorbate-induced states and overlayer metallization. More recently, we studied LT interfaces between GaAs and Mn\textsuperscript{11}, Ga\textsuperscript{11} and O\textsubscript{2}\textsuperscript{22}, and a RT interface with Ca\textsuperscript{12}. The results obtained with this group of interfaces are in full agreement with the earlier results. We attempt to establish in this paper a coherent picture of these results, to discuss them in terms of the main Schottky barrier models, and to draw some conclusions on the mechanisms which most likely induce and determine band bending at the GaAs(110) surface in various metal coverage regimes.

II. EXPERIMENTAL CONSIDERATIONS

The experiments were performed on (110) n-GaAs (1-5x10\textsuperscript{17}/cm\textsuperscript{3}) and p-GaAs (5x10\textsuperscript{17}/cm\textsuperscript{3}) surfaces cleaved in-situ. The temperature of the sample was maintained at RT or LT during metal deposition or exposure to O\textsubscript{2}, and during the measurements. Metallization was obtained by resistive evaporation of metals from W baskets. The evaporations were done in incremental coverages ranging between 10\textsuperscript{-2}ML and 10-20ML (1ML = one monolayer = 0.89x10\textsuperscript{15}atm/cm\textsuperscript{2}), and were controlled with a quartz crystal thickness monitor. Nominal thicknesses of 1ML Ga, Mn and Ca on GaAs(110) are 1.7Å, 1.1Å and 3.8Å respectively. Exposures to unexcited molecular oxygen were measured with a cold cathode gauge. Band bending at the GaAs surface was obtained from the rigid shift of the photoemission Ga-3d and As-3d core levels measured with a cold cathode gauge. Band bending at the GaAs surface was obtained from the rigid shift of the photoemission Ga-3d and As-3d core levels as a function of metal coverage. The soft X-ray photoemission spectroscopy (XPS) measurements were done at the Synchrotron Radiation Center of the University of Wisconsin. The ultra-violet photoemission spectroscopy (UPS) measurements on Ca- and O\textsubscript{2}-GaAs were done with a conventional He discharge lamp. In addition, low energy electron diffraction (LEED) and Auger electron spectroscopy (AES) were used to investigate overlayer morphology, structure and composition at some of these interfaces.