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I. Brief Technical Summary

Introduction

The original goal of this research was the study of microscopic processes at the surface of compound semiconductors. This effort developed in three major directions. Firstly, the atomic geometry of a number of III-V and II-VI compound surfaces has been studied via Low Energy Electron Diffraction (LEED) and Auger Electron Spectroscopy (AES). Although this study is still in process, a trend in surface reconstruction versus crystal bonding ionicity is likely to emerge. Secondly, we have studied the structural effects of the gas-semiconductor (in particular oxygen-GaAs(110)) interaction and have concluded to the formation of a thin amorphous layer (probably oxide) covering an ideally terminated periodic lattice. Finally, we have thoroughly studied the formation and structure of a thin metal (Al) overlayer on a semiconductor compound (GaAs(110)) and present a detailed analysis of the structure of a growing AlAs compound at the interface.

Atomic Geometry of Compound Semiconductor Surfaces

One of the features of this research has been a systematic investigation of the atomic geometry of non-polar surfaces of II-VI and III-VI compounds. The principal tool of investigation was LEED. The chemical characterization was done with AES. We completed the studies for GaAs [1,2,3], InSb [4], ZnTe [5,6], InP [7], and are presently finishing those of GaP [8], ZnS [9] and CdTe [10]. For some of these materials (GaAs [11], InP [7], CdTe [10]) we verified the independence of the (110) surface atomic reconstruction from the preparation technique (cleaved vs. polished-annealed surfaces). This result is now reinforced by analyses done on MBE grown surfaces [12]. For the most covalent (GaAs and InSb) of the four materials studied, we find that the anion rotates outward and the cation inward in a fashion such that bond lengths remain unaltered to within 1%. Moreover, these reconstructions penetrate at least two atomic layers into the surface [1,2,3]. The surface reconstruction of the more ionic ZnTe is characterized by smaller displacements of the anion species and the absence of distortion on the second and deeper layers. The structure of InP can be considered as intermediate. This study presents evidence that the structure of the (110) surface of zincblende compound semiconductors vary with spectroscopic ionicity: the difference between III-V and II-VI compounds seems to be associated with the differing local coordination chemistry of the group VI(II) vs. group V(III) elements [13] and the tendency to keep constant the length of mostly covalent bonds.

Gas-Semiconductor Interaction: Oxygen-GaAs(110)

LEED was used to investigate the structural effect of exposing a well ordered cleaved GaAs(110) to molecular and excited oxygen. This study was motivated by a number of conflicting results and interpretations

of the O-GaAs(110) system obtained mainly through photoemission experiments [14,15] and theoretical calculations [16]. In our study [17,18], the interaction was shown to disorder the first 1 or 2 atomic layers of the substrate without producing any ordered chemisorption of oxygen on GaAs(110). For a precise exposure ($5 \cdot 10^{18}$ L oxygen), the disordering process was found to be complete, leaving a thin (1-3Å) amorphous layer (probably $\text{Ga}_2\text{O}_3, \text{As}_2\text{O}_5$) on top of a perfectly undistorted substrate lattice. Exposition to excited oxygen showed that the process mentioned above is presumably a defect-induced dissociation of molecular oxygen with subsequent oxidation of the surface.

Metal Overlayers: Al/GaAs(110)

During the past few years, the microscopic geometry of metal-semiconductor interfaces emerged as a fundamental input to the interpretation of photoemission and theoretical studies of the initial steps of Schottky barrier and metal-semiconductor contact formation. Among the most investigated system is Al on GaAs((100) and (110)). Several models of Al/GaAs(110) emerged which included Al chemisorption on the surface 6a [19], Al-Ga replacement reaction in the top atomic layer [20] and Al forming 2-D metallic rafts weakly bond to an undisturbed surface [21]. Our LEED-AES studies [22,23,24,25] of thin (0.7Å-11Å) Al overlayers showed several crucial points. The room temperature deposition of 0.7-1.4Å of Al produces a mainly disordered overlayer, in disagreement with the interpretation of a Al-Ga replacement reaction. The Al-As bond strength overcomes the Al-substrate non-directional bond and favors the formation of 2-D Al raft or Al clusters. The kinetic barrier preventing a strong Al-substrate reaction is overcome by heating the system to 200-300°C. An Al-Ga replacement takes place and AlAs is grown. This LEED result is confirmed by AES [22,23] and soft X-ray photoemission [24] measurements. This result is also consistent with the larger heat of formation of AlAs compared to GaAs. For thicker overlayers (15-20Å), the structural analysis clearly shows [25] the formation of AlAs on top of GaAs(110). These results are clearly important as they provide a structural basis for the study of Al on GaAs and also perhaps AlAs-GaAs heterojunctions.

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