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Metal Overlayer Deposition on Se/GaAs(100)

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Deposition of Al and Au were performed on the Se treated GaAs(100) surface. The deposition of Al at low coverages results in a significant reduction in band bending that is interpreted as further passivation of the Se treated GaAs surface. At intermediate coverages, band bending is consistent with what one would expect based on the Schottky limit. At higher Al coverages, band bending is increased higher than expected from an ideal Al/GaAs interface. Deposition of Au results in segregation of only one Se species and provides further evidence on the structure of the Se/GaAs surface. Finally, Schottky barrier heights of 0.3 and 0.9 eV were realized for Al/Se/GaAs and Au/Se/GaAs respectively, suggesting the Se passivated surface provides a wide degree of freedom in the fabrication of GaAs based Schottky barrier diodes.

1. Introduction:

Passivation of the GaAs surface by either S or Se has been shown to impart drastic photoluminescence yield gains, increase in the current gains of GaAs hetero bipolar transistors(HBT) and in general improve the overall electrical characteristics of GaAs based devices[1]. These results all indicate that the GaAs surface state density is significantly reduced following S or Se treatment. Investigations of the chemical bonding and structure of the passivated GaAs surface have all provided insight and a deeper understanding of the passivation process on an atomic level.

While our understanding of the passivated GaAs surface has progressed rapidly in the last few years, there have been only a few reports on the changes that take place in the presence of a deposited overlayer. An understanding of these changes is critical in order to assess the ultimate effectiveness of these passivation techniques since overlayer deposition is required for the fabrication of a number of electronic and optical devices of potentially commercial importance.

In this investigation, we report on the chemical bonding changes that take place at the Se/GaAs surface following deposition of Al and Au thin film overlayers. These two metals were chosen since Al and Au have a low and high work function respectively thus giving a range in Schottky Barrier Heights for the ideal Schottky limit. Thus these two systems are at relative extremes for the variety of metals that can be considered in the fabrication of possible Schottky diodes and thus provide insight not only into the type of reactions that take place at the Se passivated GaAs surface, but provides a greater understanding of Schottky barrier formation following metal deposition.

2. Experimental:

The samples were n type GaAs wafers(Si doped) with a carrier density of 1×10^{18} cm^{-3}. The GaAs wafers were first rinsed in acetone and then purified water before dipping in a commercial alkaline based etchant for 5 minutes. Following this, the sample was rinsed in purified water and then dried with $N_2(g)$. The etched GaAs wafers were then attached to a Mo sample holder with In solder and placed in a vacuum chamber connected to both an analysis and MBE chamber.

The GaAs substrate was then heated in an As overpressure for about 5 minutes at $600^{o}C$ to desorb the surface oxides. At this stage, the characteristic 2x4 As rich structure was observed by RHEED. The substrate temperature was then lowered where the surface structure changed from 2x4 to 2x1 and placed in a combined surface analysis system located at the Photon Factory on beam line BL-1A in Tsukuba. Synchrotron Radiation Photoemission Spectroscopy(SRPES) measurements were then performed. The temperature of the substrate in all cases was measured directly by an optical pyrometer. The Se deposition was performed in a MBE chamber where the effusion cell was heated and maintained at a temperature of $150^{o}C$ during deposition while the GaAs substrate was heated at $450^{o}C$.

The synchrotron photon energy was adjusted to 120 eV for the Al/Se/GaAs system and 126eV for the Au/Se/GaAs system to obtain surface sensitive information on the Se 3d, As 3d Ga 3d, Au4f and Al 2p core levels. The incident photon energy calibration was made by directly measuring the Fermi edge of Au.

3. Results and discussion:

3.1 Al/Se/GaAs:

The initial stages of Schottky Barrier formation, and chemical bonding changes for Al on GaAs(110) and (100) has been studied quite extensively using photoemission spectroscopy by a number of investigators[2,3]. The work presented here is an attempt to understand the chemical bonding changes and

Schottky barrier formation that take place as Al is deposited on the Se treated GaAs surface.

To begin our discussion, changes in the Se treated GaAs surface as a function of Al overlayer thickness as reflected in the Ga 3d spectra are shown in Fig. 1. The Ga 3d spectrum corresponding to no Al overlayer is consistent with previous results consisting of a Ga-Se and a GaAs component. Following Al deposition, a low binding energy(BE) component assigned as metallic Ga is observed with increasing intensity near 17.5 eV and is a result of Al exchanging with Ga to form a thermodynamically stable Al_xSe_y overlayer. A similar exchange reaction has been observed for the S treated surface[4]. In addition to this reaction, the main peak energy position shifts as a function of Al overlayer thickness.

The next point worthy of discussion concerns the degree of band bending as a function of Al overlayer thickness. Band bending estimates were made on the basis of relative peak energy shifts in the As 3d position with the initial band bending determined in absolute terms from the valence band maximum position relative to Fermi edge for a standard Au reference. Initially, a band bending shift from 0.41 to 0.16 eV is observed for an Al overlayer thickness of only 1.0 Å, as shown in Fig. 2. A further reduction in band bending to 0.11 eV is observed for a 1.4 Å Al thin film. The ideal Schottky barrier height for Al on GaAs yields a band bending of 0.21 eV suggesting that an additional passivation effect is realized at these very low Al coverages. This result is also consistent with the fact that Al at this stage only bonds to Se with essentially no metallic Al residing on the surface. At intermediate coverages, the band bending increases to a value in very good agreement with the ideal Schottky limit value. This result is consistent with the observation of a metallic Al peak in this thickness regime. At an overlayer thickness exceeding 5Å, additional band bending is observed and can be interpreted as a result of surface disruption resulting from Al deposition. In contrast to the Se passivated GaAs, Al deposited directly on clean oxide free GaAs results in Fermi level pinning near 0.7-0.8eV irrespective of the work function of the metal used in the deposition. Thus for the range of thicknesses investigated here, a nearly ideal Schottky Barrier height is obtained for the Al/Se/GaAs sytstem.

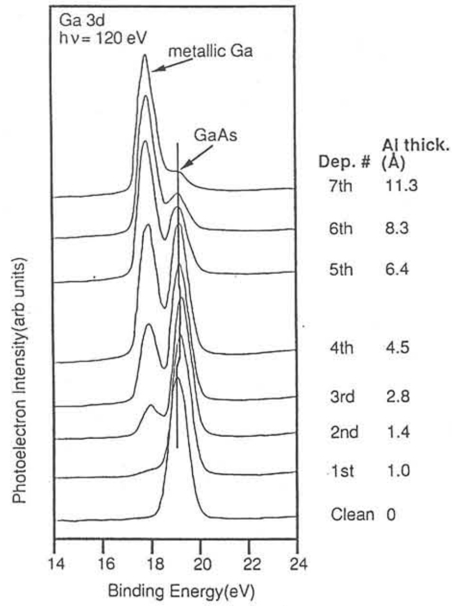

Figure 1: The Ga 3d SRPES spectra are plotted for various Al overlayer thicknesses. A metallic Ga peak is observed at low binding energy that increases with increasing Al overlayer thickness.

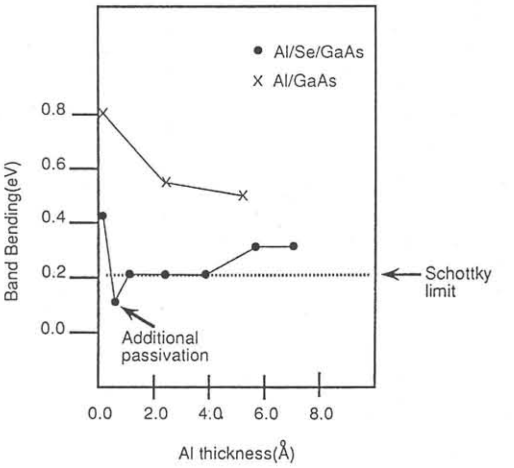

Figure 2: The band bending is plotted for Al/Se/GaAs.

3.2 Au/Se/GaAs:

The deposition of Au on the clean GaAs surface has also been thoroughly studied by a number of workers[5,6]. The discussion of this system begins by examining the changes in the As3d spectra plotted as a function of Au thickness. In contrast to Al, no evidence of metallic Ga resulting from an exchange reaction with Au is observed. The Ga 3d and Au 4f spectra were also recorded, but again no spectral changes were observed as a function of Au overlayer thickness indicating that Au does not interact significantly with any of these substrate atoms.

While no changes were observed for the Au, As and Ga spectra, drastic changes in the Se 3d spectra were observed and plotted in Fig. 3. A detailed discussion and assignment of the Se 3d spectra for the Se treated GaAs surface with no overlayer has been discussed in detail elsewhere[7-9]. The Se 3d spectra were deconvoluted into two Se species(Se(1) and Se(2)) with each species composed of a $Se3d_{3/2}$ and $3d_{5/2}$ spin orbit split component with an energy separation of 0.83eV. When Au is deposited on the Se/GaAs surface, the Se(1) species intensity increases relative to the Se(2) species as the Au overlayer thickness increases, as can be seen in Fig. 3. The degree of Se attenuation as a function of Au overlayer thickness relative to Ga and As is plotted in Fig. 4. In this plot one can see that the intensity of the Se(2) species attenuates to the same degree as As and is evidence that this species essentially remains at the Au/GaSe interface. In contrast, the Se(1) intensity is hardly attenuated indicating that this species segregates to the surface. These results suggest that the Se(1) species is located at the surface and therefore more susceptible to segregation following Au deposition and therefore provides indirect evidence of the Se assignment and recently proposed model of the Se/GaAs surface by Maeda et al.[9].

Finally, the extent of band bending as a function of Au overlayer thickness for the Au/Se/GaAs system is investigated. An initial band bending near 0.3 eV for the Se treated surface is observed. Following Au deposition, the band bending continuously increases from 0.3eV to 0.9eV as the Au overlayer thickness increases from 5 to 15Å respectively. The first point that merits discussion is that no band bending changes are observed in the thin film region(up to 5Å) indicating that no additional passivation effect is realized with Au. However, no additional band increase is observed either demonstrating that the Schottky barrier formation begins to take place only after depositing several Au monolayers. While an ideal Schottky barrier value is not attained, the results when contrasted to Al/Se/GaAs indicate clearly that there is a much greater degree in control of Schottky Barrier heights(0.6eV=0.9eV(Au)-0.3eV(Al)) when the initial GaAs surface is treated and passivated with Se than when the metals are deposited directly on the clean but unpassivated GaAs surface.

4. Conclusions:

The deposition of Al and Au on the Se treated GaAs(100) surface has provided some interesting chemical bonding observations that take place at the Se/GaAs interface. In the case of Al for low coverages, a band bending of only 0.1eV(essentially flat) is obtained and is interpreted as Al additionally passivating the Se/GaAs surface. At higher coverages, a slightly higher than ideal Schottky barrier height is obtained and correlated with segregation of Se at the Al/Se/GaAs surface. While no drastic changes in the Ga3d, As3d and Au4f spectra were observed for Au/Se/GaAs, significant changes in the Se 3d spectra as a function of Au overlayer thickness was observed. Deconvolution of the Se 3d spectra indicate that the designated Se(1) species segregates to the surface while the Se(2) species remains at the Au/Se/GaAs interface. Finally, a wide range of Schottky barrier heights for these two systems was obtained suggesting a greater degree of freedom in the fabrication of Schottky diodes can be realized with Se treated GaAs surfaces.

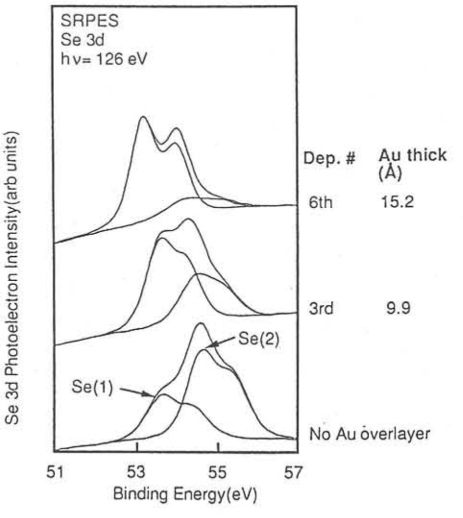

Figure 3: The deconvoluted Se 3d spectra are plotted for several Au thicknesses. One can clearly see in this plot that the Se(2) component is attenuated as the Au overlayer thickness increases. In constrast, the Se(1) component increases in intensity suggesting that this component segregates to the surface.

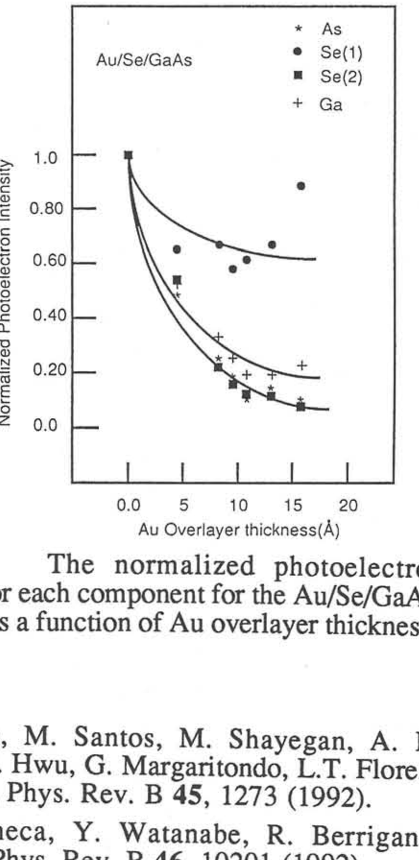

Figure 4: The normalized photoelectron peak intensity for each component for the Au/Se/GaAs system is plotted as a function of Au overlayer thickness.

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