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Synchrotron Radiation Photoemission Study on $(NH_4)_2S_x$-treated n-GaAs

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Recently it was found that the Schottky barrier height for the metal/$(NH_4)_2S_x$-treated GaAs contacts strongly depends on the metal work function.[1), 2)] This suggests that the Fermi level for the GaAs surfaces treated with $(NH_4)_2S_x$ is unpinned. However the mechanism of how $(NH_4)_2S_x$ treatment makes the surface free of pinning is not clearly understood. We investigated the $(NH_4)_2S_x$-treated GaAs surfaces using synchrotron radiation photoemission technique. In this paper the chemistry of $(NH_4)_2S_x$-treated GaAs surfaces and of the initial stage of the Schottky barrier formation on $(NH_4)_2S_x$-treated GaAs is discussed.

Photoemission spectra of Ga3d, As3d, S2p, and Al2p for n-GaAs (100) treated with $(NH_4)_2S_x$ were measured before and after the deposition of monolayer-order Al using synchrotron radiation ($h\nu$=209.4 eV) and MgKα x-ray at the Photon Factory BL-1A in Tsukuba.

Figure 1 shows synchrotron radiation photoemission spectra for $(NH_4)_2S_x$-treated GaAs surfaces. At least three bonding states including S-Ga, S-As and S-S are observed for $(NH_4)_2S_x$-treated GaAs. After the 360°C annealing in vacuum which reportedly makes the surface 2x1 reconstructed[3)], the signal intensity of S-S and S-As subpeaks decreased and S-Ga component became dominant. Therefore the sulfur atoms are thought to terminate the Ga dangling bonds, if existed, at the GaAs surfaces. The thickness of the surface GaS_x layer is determined to be about 5 Å based on the peak intensities, escape depths and photoionization cross sections. The main peak shift of both Ga3d and As3d towards higher binding energy by about 0.3 eV can be explained by a model that the upward band bending of n-type GaAs was relaxed by the formation of stable Ga-S bonds.

Next we investigated the Al/GaAs interfaces. Figure 2 shows photoemission spectra for $(NH_4)_2S_x$-treated GaAs surfaces covered with monolayer-order Al. Large metallic Ga3d and Al2p peaks are observed especially for the Al-deposited surface on 360°C-annealed GaAs. This suggests that the interfacial reaction such as Al+GaS_x $\rightarrow$ AlS_x+Ga occurs and that an Al(Ga)/AlS_x/GaAs structure is formed. On

the other hand, a large Al2p peak in the AlS_x state is observed at the Al/as-treated GaAs interface. These sulfur atoms in the AlS_x state are mainly from AsS_x. The bond breaking of Ga-S and As-S and the formation of Al-S bonds are thermodynamically reasonable, taking into account heats of formation of these sulfides. These results suggest that the interfacial Al-S bonds play an important role for the metal-dependent Schottky barrier formation. Above photoemission data are in good agreement with the I-V and C-V characteristics of the Schottky diodes.

In summary, it was found that the stable Al-S bonds at the Al/GaAs interface are the key for the unpinned Schottky barrier formation.

References

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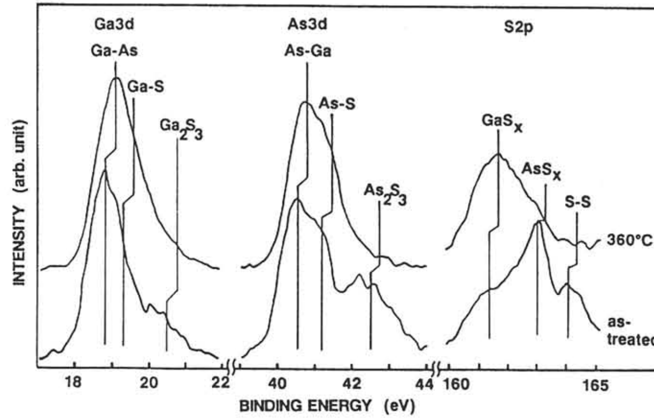

Fig. 1. Synchrotron radiation photoemission spectra for $(NH_4)_2S_x$-treated GaAs (100).

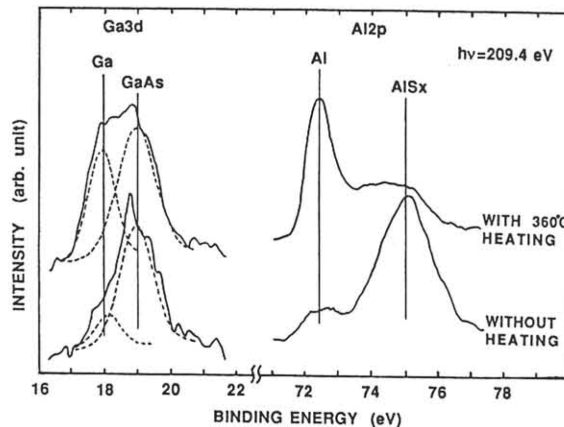

Fig. 2. Ga3d and Al2p photoemission spectra for $(NH_4)_2S_x$-treated GaAs (100) surfaces covered with monolayer-order Al.