Study of GaAs(001) Surface with Adsorbed Oxygen

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1 Introduction

The authors have investigated the effect of pretreatment by pH-controlled chemicals on Schottky barrier heights of Ni/n-GaAs junctions.[1] An X-ray photoelectron spectroscopy (XPS) analysis of the treated surface suggested that difference in surface oxygen densities is the cause of the different electrical characteristics. In order to clarify it's mechanism, electronic status of GaAs(001) surfaces with and without adsorbed oxygen atoms were studied using DV-$X\alpha$ method,[2] and compared with experimental results of Ni/n-GaAs(001) Schottky junctions.[3]

2 Results and discussion

n-GaAs(001) wafers were pretreated by HCl (pH=1) or NH_4OH (pH=13) solutions, and their surfaces were analyzed by XPS. It was found that the HCl-treated wafer has twice higher density of adsorbed oxygen and XPS spectral shapes identical with those of a bulk. After that, Ni/n-GaAs(001) Schottky diodes were fabricated and measured I–V and C–V characteristics. As a whole, the HCl-treated samples has 0.2–0.3 eV higher effective barrier heights and lower interface states than those of the NH_4OH-treated samples.

The authors calculated the electronic status of GaAs surface with adsorbed oxygen atoms in order to clarify what influence do oxygen atoms give to the GaAs surfaces. We used cluster models of GaAs(001) surface, with chalcogen atoms(O, S, Se, Te) adsorbed at the bridge site. By adsorption of chalcogen atoms on the GaAs surface, electrons shift from GaAs surface to the chalcogen atoms due to difference of electronegativities of the elements. Fig. 1 shows net charges of the adsorbed chalcogen atoms and Ga(As surface) and As(Ga surface) atoms on the GaAs(001) surface. Density of states (DOS) of Ga-terminated GaAs(001) surface is shown in Fig. 2 (a), and that of the oxygen adsorbed surface is shown in Fig. 2 (b). Without oxygens, no energy gap is seen at the GaAs surface, because dangling bond states of the top Ga layer occupy the GaAs energy gap. On the other hand, the oxygen adsorbed surface shows that the surface state density in the energy gap is remarkably reduced. It is because that oxygen-Ga bonding state lies in the GaAs valence band, and oxygen-Ga anti-bonding state lies in the conduction band. However on a As-terminated surface, oxygen adsorption increase the surface states as shown in Fig. 2 (c) and (d).

3 Discussions

A series of experimental results seem to be explainable by results of the molecular orbital claculations of O-adsorbed GaAs(001) surface.

3.1 Surface state density

From the comparison of the experimental data with the calculation results, the bare Ga-terminated portions and/or the oxygen adsorbed As-terminated portions are posturated as the cause of the surface states which degrade the electrial characteristics. While, the high density of oxygen adsorption on the Ga-terminated portion and the bare As-terminated portion are posturated as the cause of the low surface state density of the HCl-treated samples. As mentioned above, it is possible to qualitativity comprehend the results of the experiments according to consideration of effects of adsorbed oxygen atoms on GaAs surface, as summarised in Table 1.

3.2 Different Schottky barrier height

The different barrier heights can be attributed to the different density of the adsorbed oxygen. The calulation showed that the adsorbed oxygen atoms take electrons from the wafer surface, due to its so high electronegativity, and behave as negative ions. This consequently originates a dipole between the oxygen atoms and donor ions of the wafer, as the latter are the main supplier of free electrons. Then, the energy band near the semiconductor surface is bent upward as shown in Fig. 3. When the Schottky metal is formed on the treated surface, the surface oxygen atoms take electrons not only from the semiconductor but mostly from the metal. However, the influence still remains due to the high electronegativity, and a finite inter-atomic distance between the metal and the adsorbed oxygens, as indicated by $\Delta\phi$ in Fig. 3.

4 Conclusion

The authors studied influence of adsorbed chalcogen atoms (especially oxygen) on electronic states of GaAs(001) surface by using molecular orbital calculation, and compared the results with experimental results of Ni/n-GaAs (001) Schottky junctions. These calculation results qualitatively explain the results of the experiments.

References

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2. H. Adachi *et al.* : *Hajimete no densijyotai keisan*, (SANKYO SYUPPAN, Tokyo, 1997) [in Japanese].
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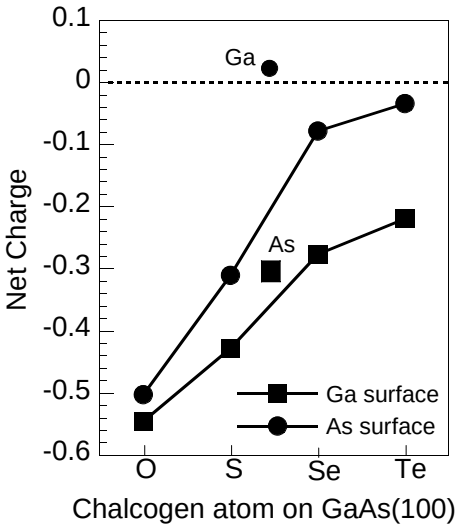

Fig. 1 Net charge of chalcogen and Ga and As atoms on GaAs(001) surface.

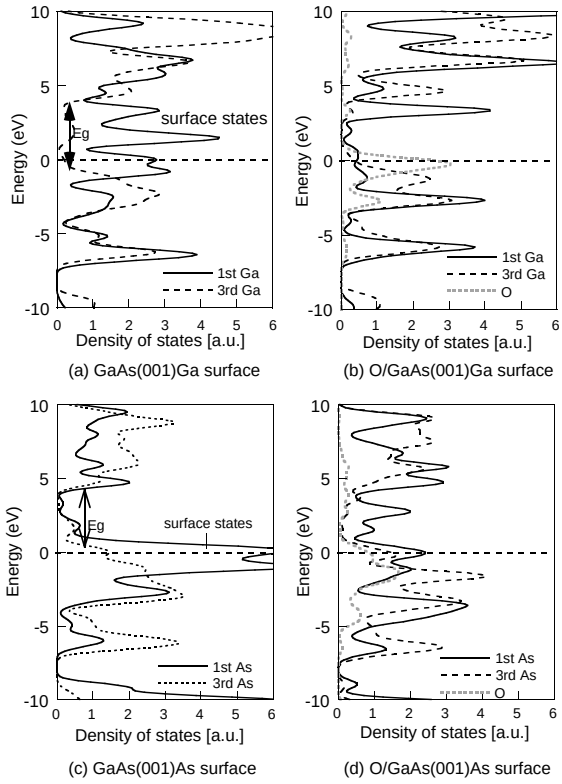

Fig. 2 Density of states of Ga-terminated GaAs(001) surface (a), oxygen adsorbed Ga-terminated surface (b), As-terminated GaAs(001) surface (c) and oxygen adsorbed As-terminated surface (d)

Table 1 Conparison of the calculation with the experimental

Calculation	Experimental
– O-Ga bond remarkably reduces the surface states in the forbidden band. – bare As-terminated surface has low density surface states.	– HCl-treated wafer surfaces have more oxygen (XPS) and low density of interface states (C–V). – No sign of O-As bond (XPS).
– bare Ga-terminated surface has high density surface states. – O-As bond increases surface states reduction.	– C–V of NH_4OH-treated wafer suggested high density of interface states. – As_2O_3 was observed although NH_4OH-treated wafer has less oxygen (XPS).
Adsorbed oxygen atoms strongly attract electrons from GaAs surface.	HCl-treated sample has higher O density and SBH* of the Ni/n-GaAs junctions as compared with the

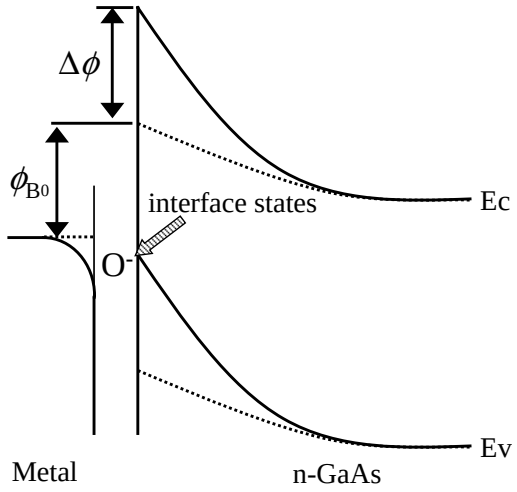

Fig. 3 Band bending in a Schottky junction on an oxygen adsorbed n-GaAs surface.