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Control of GaAs Schottky Barrier Height by Ultrathin MBE Si Interface Control Layer

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An attempt is made to control the Schottky barrier height (SBH) of the Al/GaAs Schottky barrier by inserting ultrathin MBE Si interface control layer (Si ICL). Theoretical calculation of SBH is presented based on a new model. Experiments has shown that the SBH can be varied precisely over a wide range of about 400 meV by the use of the pseudomorphic Si ICL with suitable As doping. When the Si ICL is relaxed, control becomes more difficult due to competition between the dipole resulting from ionized dopant atoms and the ionized interface states at the Si ICL-GaAs interface.

1. Introduction

Schottky junctions find applications in many advanced solid-state devices including Schottky TTL circuits, GaAs MESFETs, millimeter and submillimeter diodes and future quantum devices. Thus, artificial control of the Schottky barrier height (SBH) is an interesting possibility to be explored. Obviously the issue is closely related to controllability of the so-called "Fermi level pinning" phenomenon. Based on the DIGS model concerning Fermi level pinning[1], we proposed use of an ultrathin MBE Si interface control layer (Si ICL)[2] and succeeded in complete unpinning at InGaAs surfaces[3].

The purpose of this paper is to apply our Si ICL technique to control the SBH of the Al/GaAs Schottky barrier. It is shown that the SBH can be varied precisely over a wide range of about 400 meV by the use of the Si ICL with optimum thickness and suitable doping.

2. Basic Concept of SBH Control by Si ICL

The basic structure to control the SBH is shown in Fig.1(a). In this structure, the thickness of the Si ICL is kept to be very thin (0 - 40Å) so as to make it transparent for tunneling electrons or holes. Since the Si ICL is much thinner as compared to the thickness of the GaAs depletion layer, the GaAs band can be approximated to be flat in the vicinity of the interface region, as shown in Fig.1(b).

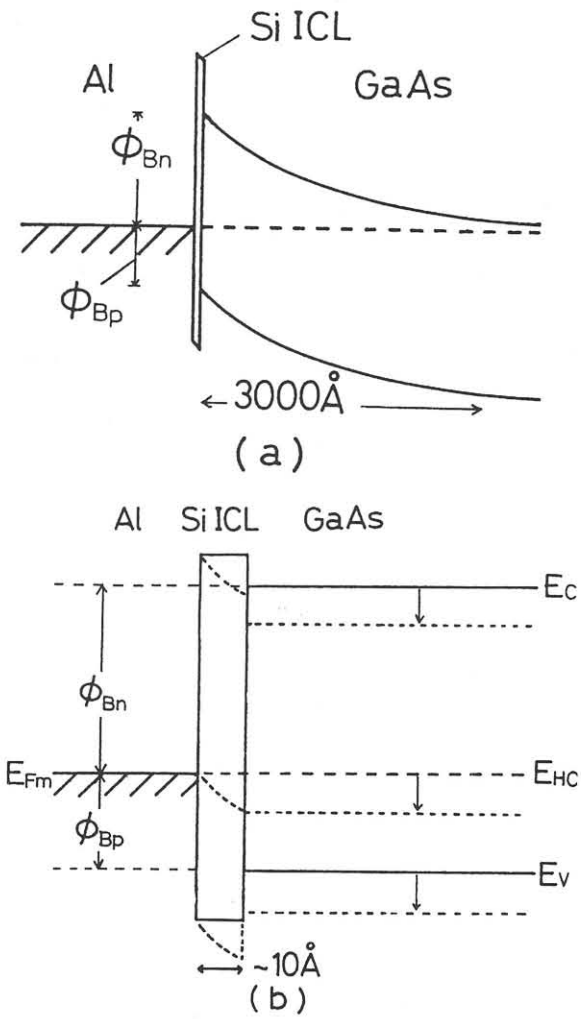


Fig.1 (a) Sample structure and (b) the band diagram near the interface region.

The structure in Fig.1(a) has two interfaces, namely, the metal-Si ICL interface and the Si ICL-GaAs interface. Based on the DIGS model for Fermi level pinning[1], we assume that a strong Fermi level pinning takes place at former interface, whereas the interface Fermi level at the latter interface remains unpinned if the ultrathin Si layer remains pseudomorphic with respect to the underlying GaAs.

Then, when the Si ICL is undoped, the band diagram becomes as shown be the solid lines in Fig.1(b). This is because both of the pinning at the metal-Si ICL interface and the band alignment at the Si ICL- GaAs take place at the hybrid orbital energy[1], E_{HO} or Tersoff's midgap energy[4] of GaAs, lying at 0.47 eV above E. Then, the SBHs for electrons and holes are given by (E_C - E_{HO}) and (E_{HO} - E_V), respectively

When the ICL is doped to a sufficiently high level, the high field resulting from ionized impurity atoms will modify the SBH, even if the ICL thickness is extremely small. Thus, when the Si ICL is highly doped to n-type,the SBH for electrons is reduced and that for holes is increased, as shown by the dashed lines in Fig.1(b). When the ICL is doped to highly p-type, the contrary situation takes place. To cause significant changes of the SBH, the ICL should maintain good crystalline order with respect to GaAs and, at the same time, its maximum doping level should be at least in the range of10^{20} cm^{-3}. Si was chosen as a possible candidate to meet these two requirements.

3. Theoretical Calculation of SBH

Based on the above concept, theoretical calculation of SBH was made by solving the Poisson's equation. Examples of the results of calculation are shown by solid curves in Fig.2(a) and (b) for two cases. Figure 2(a) is for the case where no interface state exist at the Si ICL- GaAs interface and Figure 2(b), for the case where uniformly distributed interface states exist at the interface respectively.

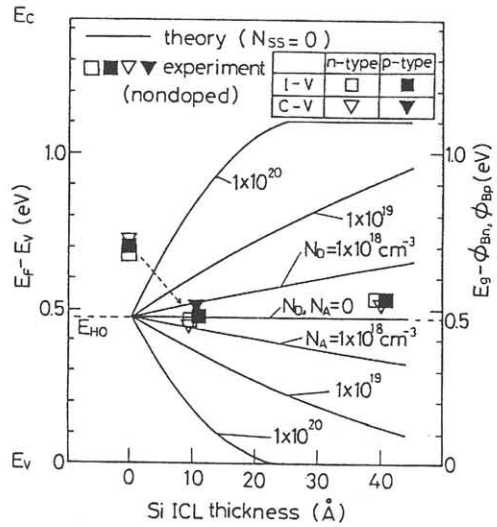
It seen from Fig.2, (a) and (b), that high doping can produce large changes of SBH, and that interface states at Si ICL-GaAs interface should be minimized to realize such large changes.

4. Experimental

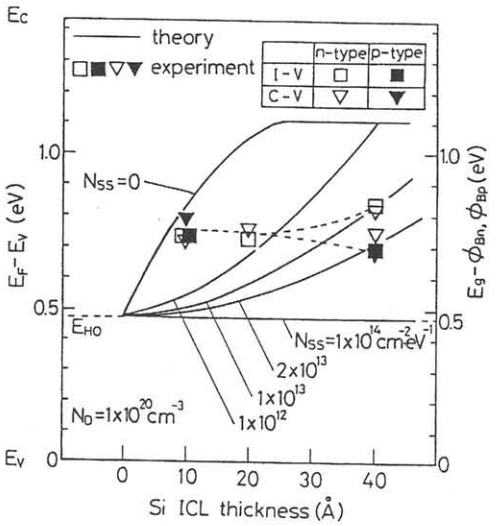
Experiments were done using a UHV system where MBE, XPS and metal deposition chambers were connected by a UHV transfer chamber. By using this system, in-situ preparation of the samples and their in-situ XPS characterization were possible.

To prepare samples, MBE growth of Si doped or Be doped GaAs with (100) orientation and the carrier concentration of about $3x10^{16}cm^{-3}$ was done at first. Then, MBE growth of Si ICL was made from Si K-cell. The substrate temperature was kept at 250 °C during the growth of Si ICL. The growth rate of Si ICL was 20 Å/hour. Doping to the Si ICL was made by As and Ga both from the K-cells.

Starting from the As stabilized (2x4) pattern of MBE GaAs, RHEED pattern quickly changed and maintained to be either (1x2) or (3x1) pattern during the Si ICL growth, depending on whether the growth was done without As-supply or under the As stabilized condition, respectively.



(a)



(b)

Fig.2 Calculated values of the SBH in terms of the Fermi level pinning position. Experimental data are also included. (a) undoped and (b) As-doped.

Finally, Al electrode was deposited either from Al K-cell in the MBE chamber, or from a tungsten resistance heater in the metal deposition chamber.

5. Results and Discussion

The Fermi level position (E_F) of Si-ICL/GaAs structure before metal deposition, as determined by the XPS core level shifts, is shown in Fig.3. The position was different, depending on the conduction type of GaAs and the type and level of As doping into Si ICL. However, no change was observed for Ga doping. This indicates that As is active as donor, but Ga is not active for some reason.

Upon deposition of metal, E_F became the same for n- and p-type samples having the same preparation conditions. Al/GaAs Schottky barriers without Si ICL showed commonly observed SBH Values of 740-760meV for n-type. By inserting an undoped Si ICL, it could be reproducibly increased up to 980 meV, as shown by the data points included in Fig.2(a).

By doping As into Si ICL to different doping levels under As-stabilized conditions, SBH could be precisely controlled over 600-980meV for n-type, and over 450-830meV for p-type samples as shown by the data points included in Fig.2(b), covering an overall change of about 380meV. On the other hand, no change of SBH was observed for Ga doping in consistent with the result prior to metal deposition.

The SBH value was very reproducible and the ideality factor n was close to unity ($n<1.05$), as long as the Si ICL was about or below 10 A. According to our previous experiment, Si ICL remains pseudomorphic up to about 10 A[3]. However, as the ICL thickness was further increased into the relaxed region, scatter of the SBH data(100meV) took place together with the appearance of discrepancies in SBH between C-V and I-V techniques. A marked increase of ideality factor ($n=1.03-2.15$) also started to take place.

By comparing the experimentally observed SBH with the theoretical values in Fig.2 (a) and (b), As doping can reproducibly change the SBH in a controlled fashion provided that the Si ICL remains pseudomorphic. Large deviations of SBH from the curve for $N_{SS} = 0$ in Fig.2(b), indicates that high densities of interface states are introduced at the Si ICL-GaAs interface when the ICL thickness is too large and the ICL is relaxed producing many misfit dislocations.

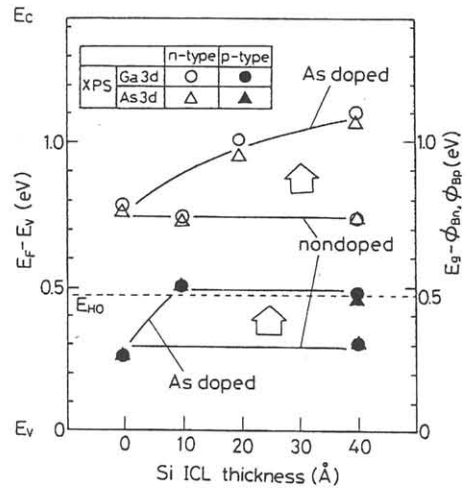


Fig.3 Initial Fermi level positions before metal deposition.

Thus all the present data can be explained quantitatively in terms of the initially stated basic concept based on the DIGS model for Fermi level pinning. Namely, a firm pinning does exist at metal-Si ICL interface whereas the Si ICL-GaAs interface becomes pinning-free or moderately pinned by interface states, depending on whether the Si ICL is pseudomorphic or relaxed. Strong dipole resulting from ionized dopant atoms changes SBH in competition with the interface state charge at the Si ICL-GaAs interface. The new model is entirely different from the mechanism involving Fermi level unpinning proposed by Grant et al in their pioneering work[5] or more recent similar works by a different group[6,7].

6. Conclusion

The Si ICL technique was applied to control the SBH of the Al/GaAs Schottky barrier. It was shown that the SBH can be varied precisely over a wide range of about 400 meV by the use of the Si ICL with optimum thickness and suitable As-doping.

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