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In-Situ UHV Study on Correlation between Microscopic Surface Structures and Macroscopic Electronic Properties in Si Interlayer-Based Surface Passivation of GaAs

Morimichi Mutoh, Naohiro Tsurumi, Tamotsu Hashizume, Hideki Hasegawa

Research Center for Interface Quantum Electronics, and Graduate School of Electronics and Information Engineering, Hokkaido University, Kita-13, Nishi-8, Sapporo 060-8628, Japan
Phone: +81-11-706-7174, Fax: +81-11-716-6004, e-mail: mutoh@ryouko.rciqe.hokudai.ac.jp

1. Introduction

High-density surface states on compound semiconductors are known to cause problems in electronic and optical devices. Although numerous attempts to form various insulators directly on GaAs for surface passivation have been made, none of them have been sufficiently effective.

We proposed insertion of an ultrathin Si interface control layer (Si ICL) between GaAs and insulator, and demonstrated its effectiveness[1]. The latest version of this passivation method is shown in **Fig. 1** where a significant improvement due to quantum confinement has been achieved by reducing the thickness of Si ICL through its partial nitridation by ECR N_2 plasma[2].

In order further to optimize this Si ICL based passivation method for GaAs, the present paper studies correlation between microscopic surface structures and macroscopic electronic properties by UHV STM, XPS, UHV contactless C-V and UHV PL methods. To change microscopic surface structures, the reconstruction of the initial GaAs surface was carefully controlled.

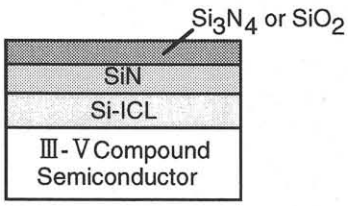

Fig.1 Si ICL-Based Surface Passivation Technique

2. Experimental

In this study, a UHV-based multi-chamber system was used where MBE chamber, ECR plasma chamber, XPS chamber, UHV-STM chamber, UHV contactless C-V chamber and UHV-PL chamber are connected by a UHV transfer chamber together with other chambers.

For sample preparation, Si-doped (2x4) GaAs layers with carrier concentration of 1-3 x 10^{16} cm^{-3} were grown on n^+ GaAs (100) substrates at substrates temperature of 580℃ in the MBE chamber. Then, the initial surface reconstruction was controlled in the following way. Namely, the initial (2x4) surface-phase could be maintained during cooling process down to the temperature of 300℃ for growth of Si interlayer, by gradually reducing the intensity of the As_4 flux. On the other hand, without reducing the intensity of the As_4 flux during cooling, c(4x4) reconstructed surfaces were obtained. Then, an ultrathin Si layer (2-10Å) was grown on these two kind of GaAs surfaces by MBE. Finally, the Si surface was partially nitrided by exposing the surface into ECR N_2 plasma at room temperature for 10s-30s.

Each step of passivation was characterized in-situ in UHV. Microscopic structural properties of the sample surfaces were studied using UHV-STM system (JEOL JSTM-4600). Electronic properties of the sample surfaces were investigated by UHV-PL and UHV contactless C-V methods. **Figure 2** shows the principle of the UHV contactless C-V method. Piezo-mechanism control with the capacitance feedback from the parallelism electrodes can realize a ultra-narrow "UHV-gap" (100-300nm) between the field electrode and the sample surface[3].

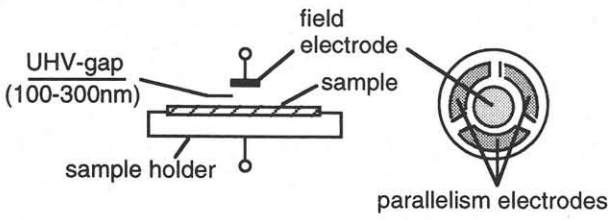

Fig.2 Contactless UHV C-V system

3. Results and discussion

Figures 3 and 4 show changes in RHEED patterns before and after 2Å-Si growth. As seen in Fig.3, the initial (2x4) pattern changed to (2x1) pattern, whereas c(4x4) surfaces changed to asymmetric (3x1) structure in accordance with a previous result[4]. Thus, different initial surface reconstructions of GaAs lead to different Si atom arrangements.

Figure 5 shows the STM images taken from the surfaces after 2-Å Si deposition. (2x1) and (3x1) microscopic structures were actually found on the initially (2x4) and c(4x4) surfaces respectively, being

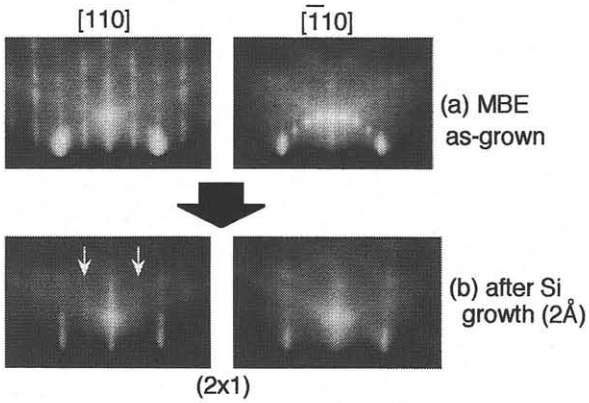

Fig.3 RHEED patterns of (2x4) surfaces

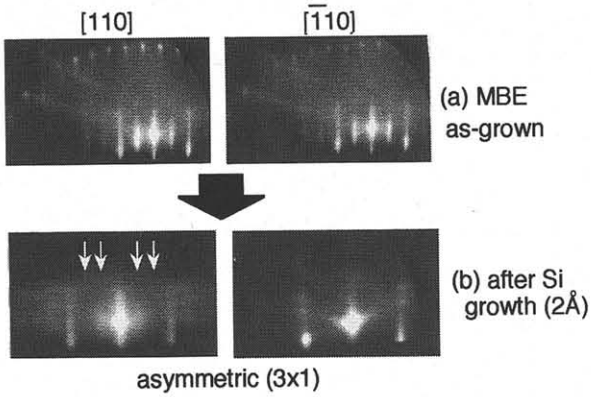

Fig.4 RHEED patterns of c(4x4) surfaces

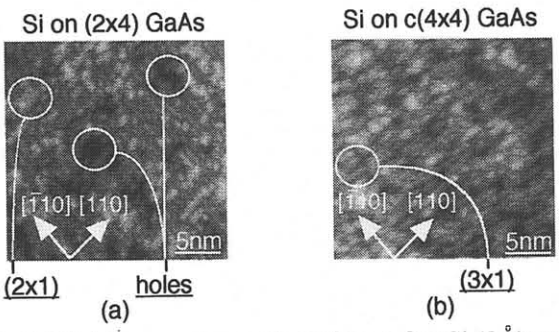

Fig.5 STM images of sample surfaces after Si (2Å) growth

consistent with the RHEED observation. Many holes were found to exist after Si deposition on the initially (2x4) surface, as seen in Fig. 5(a), whereas no holes existed and atom arrangements were much more regular on the initially c(4x4) surface. RMS values of surface flatness for the initially (2x4) and c(4x4) surfaces after Si deposition was 0.17nm and 0.11nm, respectively.

The XPS Si2p spectra after Si layer formation and the subsequent partial nitridation by ECR N_2 plasma were shown for the initially (2x4) surface in **Fig. 6**. Formation of Si-Si bonding on GaAs surfaces was confirmed by the XPS spectrum shown in Fig. 6(a). As seen in Fig. 6(b), Si nitride component was created on the surfaces after ECR N_2 plasma process. The angle-resolved XPS analysis clearly showed that only the upper part of Si layer was nitrided. These surface chemical status was found to be more or less the same for the initially c(4x4) surface.

Figure 7 shows the measured UHV contactless C-V curves of the as-grown and passivated surfaces. On the as-grown GaAs surfaces after MBE, almost flat C-V curves were obtained for both of c(4x4) and (2x4) surfaces, indicating occurrence of strong Fermi level pinning. A very limited variation of the capacitance was observed for the initially (2x4) surface even after passivation with Si interlayer and the partial nitridation. On the other hand, a larger capacitance variation was obtained on the initially c(4x4) surfaces after passivation, as shown in Fig.7 (c). Corresponding difference was also observed in the changes of PL intensity as shown in **Fig. 8**.

The present results show that the difference in the microscopic surface structure resulting from the initial

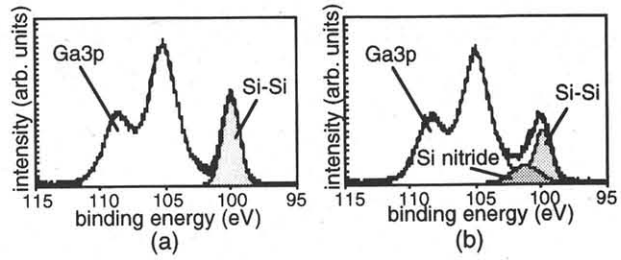

Fig.6 Si2p XPS spectra of the samples (a) after Si growth (10Å) and (b) subsequent nitridation

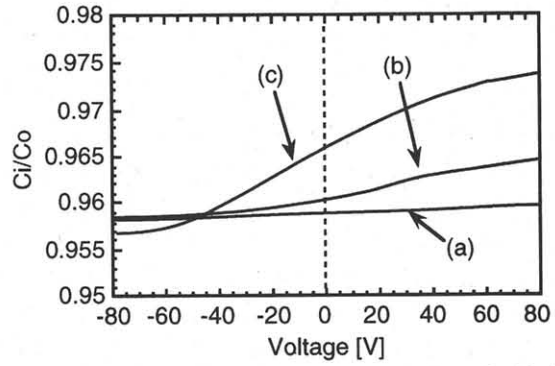

Fig.7 C-V curves of (a) MBE as-grown (2x4) and c(4x4) surfaces, (b) (2x4) after Si ICL growth and nitridation, and (c) c(4x4) after Si growth and nitridatiion

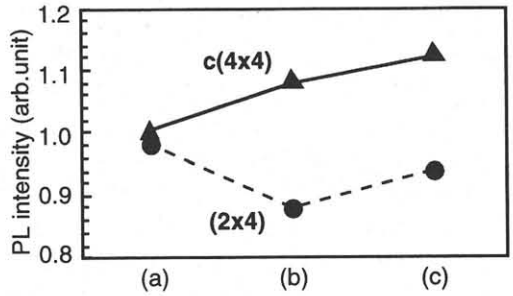

Fig.8 Changes in PL intensity of (a) MBE as grown surfacees, (b) the surfaces after Si growth and (c) the surfaces after nitridation

surface reconstruction of GaAs sensitively affects the macroscopic electronic properties after the Si ICL-based passivation. The result seems to indicate the importance of the 2-dimensional order on the Si-deposited surfaces in microscopic scale for successful passivation in support of the DIGS model[5] for Fermi level pinning. Thus, further improvement should be possible by further process optimization.

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