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In-Situ Contactless Characterization of Microscopic and Macroscopic Properties of Si-Doped MBE-Grown (2x4) GaAs Surfaces

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1. Introduction

High-density of surface states are known to cause Fermi level pinning at III-V compound semiconductor surfaces on a macroscopic scale, and make the control of surface difficult. Although there are various models, the microscopic origin of the Fermi level pinning has not been well established. On the basis of UHV-STM study, Pashley et al.[1,2] have recently proposed that kinks on missing dimer arrays on the (2x4)-reconstructed Si-doped n-GaAs surface act as acceptors and cause Fermi level pinning.

The purpose of this paper is to correlate macroscopic electronic properties of the MBE-grown Si-doped n-type GaAs (001) (2x4) surfaces with microscopic atomic structures in order to see the validity of the model by Pashley et al. Ultra-high vacuum (UHV) contactless capacitance-voltage (C-V), UHV-photoluminescence (PL) and UHV-scanning tunneling microscope (STM) techniques were used. It is concluded that the observed macroscopic pinning behavior cannot be explained by the kink-acceptor model.

2. Experimental

In this study, a UHV-based multi-chamber system shown in **Fig.1** was used where a solid source MBE chamber, contactless UHV C-V chamber, UHV-PL chamber and UHV-STM (JEOL JSTM-4600) chamber are connected by a UHV transfer chamber together with other chambers. The base pressure of each chamber as well as the transfer chamber was within the range of 10^{-10} Torr.

Samples were prepared in the MBE chamber. After the MBE growth of Si-doped GaAs, the samples were annealed in an arsenic flux for 3-10 minutes for stabilization of (2x4) ß-phase. Then the MBE layers were cooled down to room temperature with gradually reducing the intensity of the As_4 flux, maintaining (2x4) ß-phase pattern which possessed a clear Laue circle and a strong 2/4 fractional order streaks in the $[\bar{1}10]$ direction at room temperature.

Microscopic properties of the sample surfaces were studied using STM chamber, and their macroscopic electronic properties were measured by using contactless UHV C-V and PL chambers. In the contactless UHV C-V system schematically shown in **Fig.2**, the metal field plate with an area of 7.5×10^{-3} cm^2 is placed above the sample surface, keeping an ultrathin and constant "UHV-gap" (100-300nm) with the aid of a piezo-electric feedback of capacitance. Thus, *in-situ* MIS C-V assessment of "free" surfaces in UHV environment became possible for the first time. This system was checked using a standard SiO_2/Si MOS capacitors. The gap distance was determined by the optical method utilizing the Goos-Haenchen effect. The measure-ment frequency was 500kHz.

In the UHV-PL chamber, the quantum efficiency of room temperature PL from the sample was measured as a function of the incident photon flux intensity, ϕ, and the result was analyzed by the theory of the PL surface state spectroscopy (PLS^3) developed by Saitoh et al.[3]

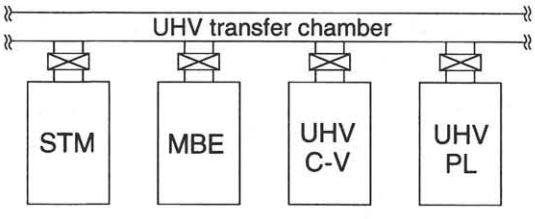

Fig.1 UHV multi-chamber system.

3. Results and discussion

3.1 Microscopic properties

Typical STM images taken on the (2x4) ß-phase surfaces of Si-doped GaAs is shown in **Fig.3** for two doping levels of 3.0×10^{17} cm^{-3} and 1×10^{18} cm^{-3}. Kinks were observed, and its density was larger at higher doping levels.

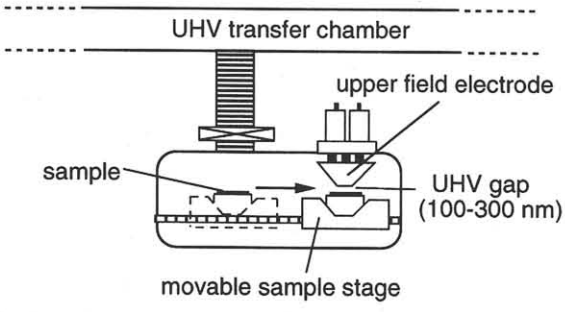

Fig. 2 Schematic illustration of UHV contactless C-V system

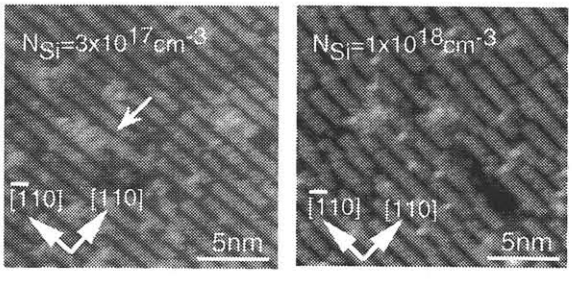

Fig.3 STM images of MBE-grown (2x4) β surafces

The relationship between the Si doping concentration and the kink density as measured on the (2x4) ß-surface is shown in **Fig.4**. The kink density increased monotonically with the Si doping concentration, in agreement with the previous work[1,2].

3.2 Macroscopic electronic properties

Figures 5 shows the measured C-V curves of the samples with the Si doping concentration of $5x10^{16}$ cm^{-3} and $3x10^{17}cm^{-3}$. Very limited variation of capacitance was observed in both samples, indicating the presence of strong Fermi level pinning whose strength is almost independent of Si-doping concentration. From the flattening values of capacitance, the pinning position is estimated to be at around $E_v + 0.6$.

Figure 6 shows the result of the *in-situ* UHV-PL measurement. The slope of the PL efficiency was found to be much smaller than unity.

3.3 Discussion

According to the kink-acceptor model, a high density of kinks pin the surface Fermi level at the energy position of the kink deep acceptor which is assumed to lie near mid-gap, as schematically shown in **Fig.7 (a)**. In this case, one should obtain a C-V curve schematically shown in **Fig.8** where the flat-capacitance region with the width of ΔV_F corresponds to filling of surface deep acceptors. For the surface with Si-doping density of $3x10^{17}$ cm^{-3}, such V_F was estimated to be 25 V using a value of kink density of $3x10^{11}$ cm^{-2} shown in Fig.4. However, the measured C-V curve showed ΔV_F>120V.

As for the PL, the PLS[3] theory [3] tells that a straight log (I_{PL}/ϕ) vs. logϕ line with a slope of unity corresponds to discrete deep level states as assumed in the kink-acceptor model. However, the measured slope is much smaller than unity and this indicates that there exists a high-density surface states with a steeply U-shaped distribution as schematically shown in **Fig.7(b)**.

Thus, the observed macroscopic C-V and PL behavior cannot be explained by the kink-acceptor model, but it indicates Fermi level pinning by a steeply U-shaped continuous surface states. We argue from the viewpoint of the disorder-induced gap state (DIGS) model that loss of two-dimensional order on the surface due to presence of missing atoms, holes, steps, etc. may create surface states of continuous nature, and cause pinning. Kinks may contribute to enhance disorder in such a context.

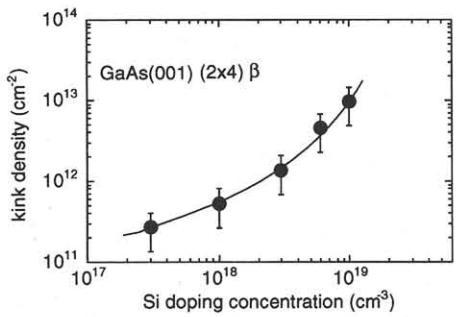

Fig.4 Kink density as a function of Si-doping concentration

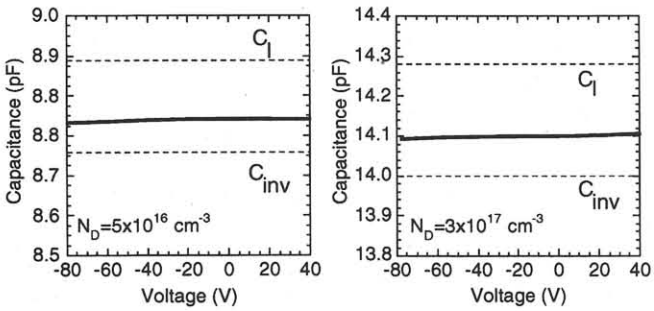

Fig.5 Contactless C-V curves obtained from the MBE-grown GaAs

References

1) M. D. Pashley et al.: Phys. Rev. B 48, 4612 (1993).

2) M. D. Pashley, K. W. Haberern and R. M. Feenstra: J. Vac. Sci. Technol. B 10, 1874 (1992).

3)T. Saitoh, H. Iwadate and H. Hasegawa, Jpn. J. Appl. Phys. **30,** (1991) 3750(1991) .

4) H. Hasegawa and H. Ohno: J. Vac. Sci. Technol. B4, 1130 (1986).

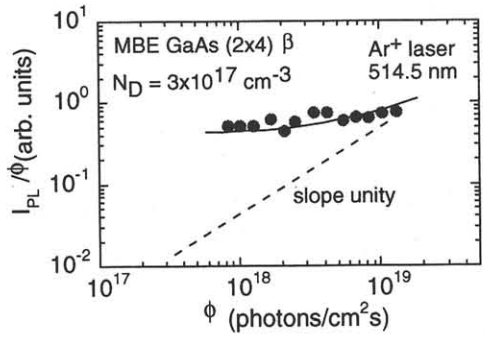

Fig.6. PL efficiency vs excitation photon flux density

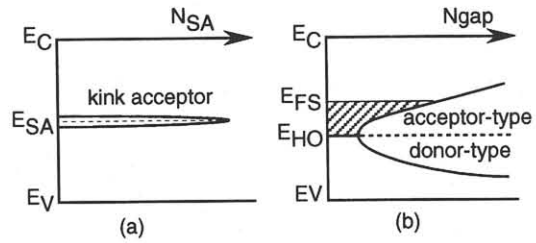

Fig. 7 (a) Kink-acceptor model and (b) U-shaped gap state model

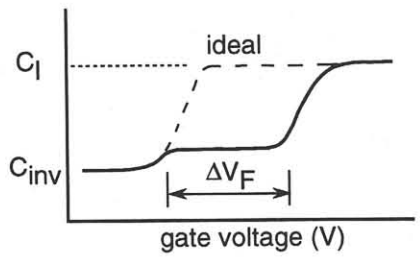

Fig. 8. C-V flattening behavior with a kink density of $3x10^{11}$ cm^{-2}