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Disorder Induced Gap State Model for Anomalous C-V Carrier Concentration Profiles at Epitaxially Grown Interfaces

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Anomalous depletion/accumulation (D/A) carrier concentration profiles were observed at GaAs/GaAs and InGaAs/GaAs MOVPE regrown interfaces prepared under various growth and processing conditions. Based on a detailed C-V and DLTS study, a disorder induced gap state (DIGS) continuum due to interface crystalline disorder rather than specific discrete deep levels is proposed to be responsible for the anomalous D/A profile and Fermi level pinning.

1. Introduction

Sharp and controlled variation of carrier concentration at the homo- or hetero- epitaxial interface is one of the essential requirements for construction of modern electronic and optoelectronic devices. However, certain epitaxial interfaces, particularly MBE and MOCVD interfaces regrown after atmospheric exposure, often show anomalous C-V carrier concentration profiles including either carrier depletion or accumulation or both near the interface[1-4] that are apparently not related to any intentional doping. So far such anomaly has been attributed to unintentional incorporation or redistribution of specific shallow or deep impurities or formation of discrete deep defect levels during crystal growth.

This paper presents the result of a detailed C-V and DLTS study on GaAs/GaAs and InGaAs/GaAs MOVPE regrown interfaces prepared under various growth and processing conditions. Anomalous carrier depletion /accumulation (D/A) profiles were detected by C-V profiling. The DLTS study indicated presence of a gap state continuum rather than discrete levels. These observations led to a new model for unoptimized epitaxial interfaces where the interface crystalline disorder introduces a characteristic disorder induced gap state (DIGS) continuum. Recently, such a DIGS model was proposed for unified understanding of metal-insulator and insulator-semiconductor interfaces[5]. The present work indicates that the unified DIGS model is also useful for understanding the anomalous depletion/accumulation C-V carrier concentration profile and Fermi level pinning at epitaxial homo- or hetero- semiconductor-semiconductor interfaces.

2. Experimental

A standard vertical MOVPE reactor was used for formation of GaAs/GaAs and InGaAs/GaAs regrown interfaces. The growth was carried out using TMG, TMI and arsine. Typical III to V mole ratio, growth rate and background carrier concentration were 1:20, 500 Å / min. and 1-2 x 10^{16} cm^{-3}, respectively. The substrate for growth was (100) oriented n^+ GaAs.

C-V profiling was done at 1 MHz on Au Schottky diodes containing regrown interfaces. DLTS measurements were done for 50-400 K on the same diodes and the detection sensitivity of the system was 5×10^{-4} - 1×10^{-3} in terms of fractional capacitance variation.

3. Experimental Results

GaAs/GaAs interfaces where growth was interrupted and resumed after various processing showed different C-V carrier concentration profiles whose phenomenological details have been discussed in detail elsewhere[3]. In particular, exposure to air was found to result in a characteristic anomalous D/A profile which was difficult to explain by any straightforward model. A typical C-V characteristics of such an interface is shown in Fig.1 and the resultant carrier concentration profile is shown in Fig.2. Similar profiles have been reported in the MBE growth[1,2,4]. Removal of native oxide before regrowth did not remove the anomaly. The anomalous profile extends widely on both sides of interface and is difficult to understand by impurity incorporation/redistribution.

It was then found that $In_xGa_{1-x}As/GaAs$ interfaces (x = 0.02 - 0.05) where the growth was interrupted only during the change of gas mixture without any exposure to air also showed very similar anomalous D/A profiles as shown also in Fig.2. This clearly shows that such a profile is not unique to oxygen exposure.

The DLTS measurements performed on the GaAs/GaAs and InGaAs/GaAs interfaces with anomalous D/A profiles shown in Fig.1, detected extremely broad spectra that were continuous in energy but spatially localized at the interface, as shown in Figs.3 and 4 for a GaAs/GaAs interface exposed to air. Figure 3 shows the bias swing dependence of the DLTS signal,

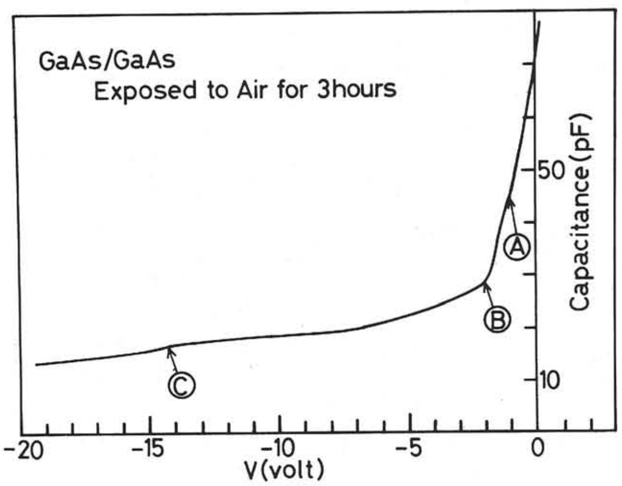

Fig.1 Schottky C-V curve for regrown interface.

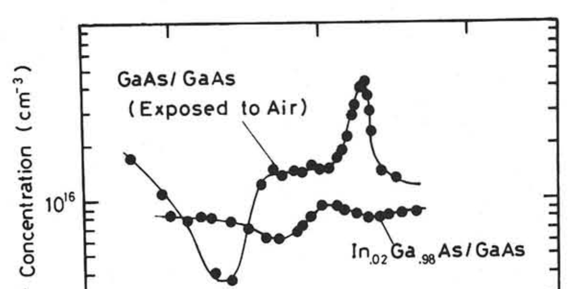

Fig.2 Anomalous D/A profiles as obtained by the C-V method

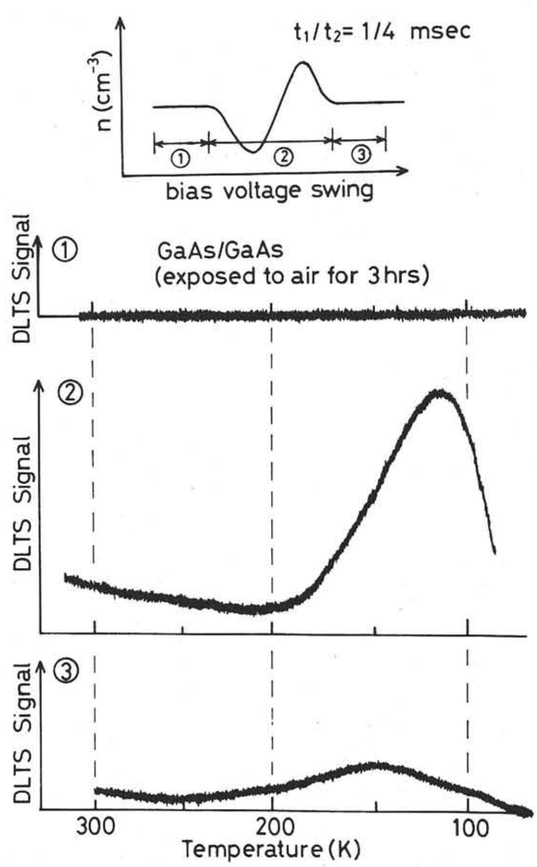

Fig.3 DLTS spectra of an air-exposed GaAs/GaAs interface as the bias swing is varied.

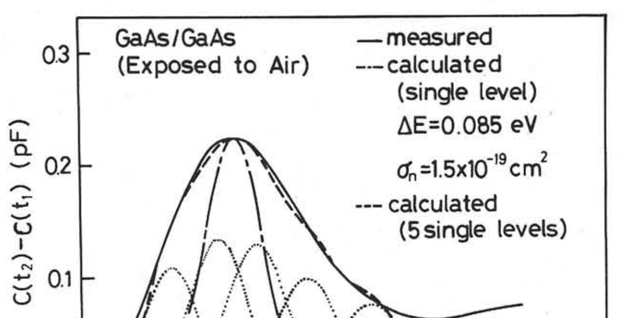

Fig.4 Shapes of DLTS response for an air-exposed GaAs/GaAs interface.

indicating that the presence of deep levels is spatially limited in the interface region. A small response in the bottom trace can be attributed to the so-called λ effect. The shape of the experimentally observed DLTS signal is compared with the theoretical curves in Fig.4. The measured response was much broader that a theoretical single level response curve whose activation energy and cross-section were determined from the Arrhenius plot of the response peak. On the other hand, use of as many as five single levels instead of one, for example, still can reproduce only a part of the response, as shown in Fig.4. The result shows that the levels essentially form a continuum rather than being discrete.

4. Disorder Induced Gap State Model

The important question is whether the observed anomalous C-V D/A profile and the interface state continuum are correlated or not. We propose here that they are indeed correlated to each other as schematically shown in Fig.5. In correspondence with Fig.1, three Schottky C-V

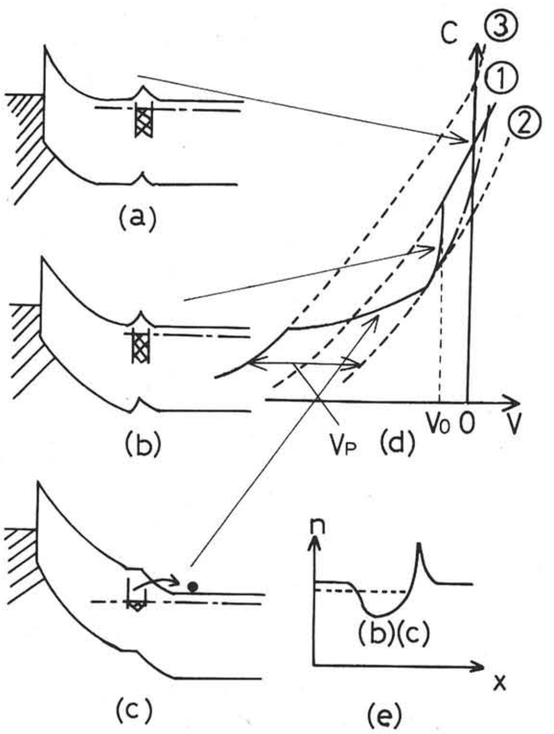

Fig.5 A new interpretation of the Schottky C-V curve.(a)-(c) band diagrams, (d) C-V curve, and (e)apparent profile.

curves①-③having the same background doping are shown in Fig.5(d) among which the actual C-V data moves around. According to our interpretation, "depletion"(Ⓐ to Ⓑ in Fig.1 and the band diagram in Fig.5 (b)) arises from the notch in the conduction band due to the filling of the interface state continuum, resulting in a rapid shift from Curve ① to ② in Fig.5(d). A more detailed band diagram of the notch is shown in Fig.6. On the other hand, "accumulation" (Ⓒ to Ⓓ in Fig.1 and Fig.5(e)) is a measurement artifact caused by escape of

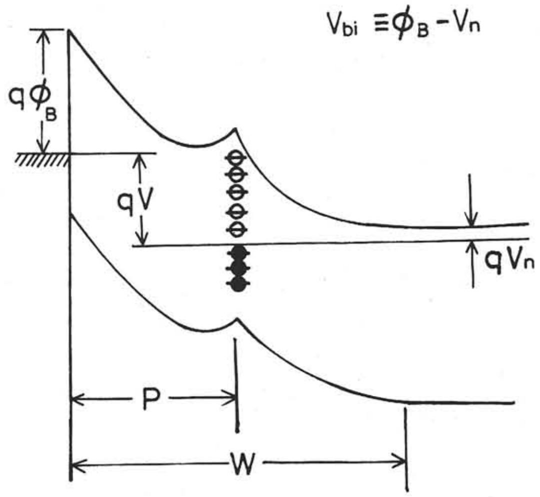

Fig.6 Band diagram showing a notch.

electrons from the interface states, resulting in a "flatband voltage shift V_p from Curve ② to ③ (without escape, the data would have stayed on Curve ②). If the regrown top layer is too thin, it is depleted from the beginning so as to result in the dash-dot curve in Fig.5(d) which may be interpreted as only accumulation being occurring.

In both depletion and accumulation, the carrier concentration by the C-V analysis is not the true concentration. Referring to Fig.6, "apparent accumulation" is given for instance by

$$dC^{-2}/dV = 2/q\varepsilon N_D(1 + (q^2N_{IS}/\varepsilon)P(W-P)/W) \quad (1)$$

where N_{IS} is the interface state density. The fact that C-V data is shifted beyond the original Curve ① towards Curve ③ during electron escape in Fig.5(d), indicates that both acceptor and donor states exists.

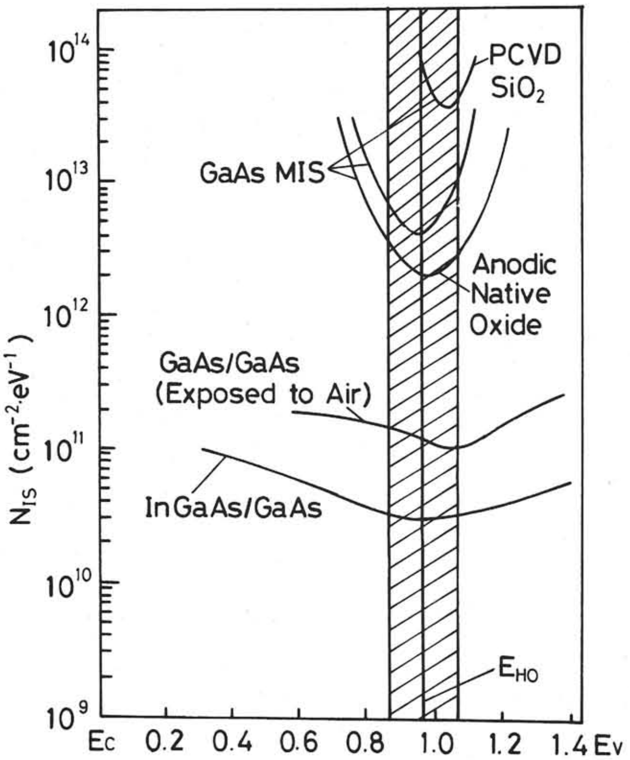

Fig.7 Measured interface state distributions of regrown interfaces and MIS interfaces[5].

The interface state distributions based on a rigorous C-V analysis (Terman's method as modified to the present system) are summarized in Fig.7 together with some results on MIS systems[5]. The shape and magnitude of the distributions were found to be consistent with the results of the DLTS measurement. In Fig.6, U-shaped interface state continuum is seen whose minimum falls near the Fermi-level pinning position of Schottky barrier and N_{SS} minimum position of insulator-semiconductor interfaces.

The origin of the interface state continuum can be explained by the unified disorder induced gap state model recently proposed for insulator-semiconductor and metal-semiconductor interfaces[5]. Formation of thin oxide, loss of stoichiometry, lattice mismatch etc. produce interfacial disorder which introduces a disorder induced gap state (DIGS) spectrum in the gap as shown in Fig.8. The charge neutrality point of DIGS spectrum has been found to be given by the hybrid orbital energy E_{HO} of the sp^3 bond[5]. Although the DIGS density depends on the degree

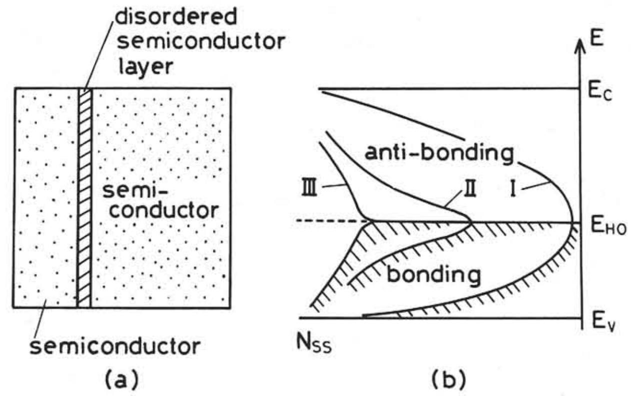

Fig.8 Disorder induced gap state (DIGS) model for unoptimized epitaxial interfaces. I,II and III correspond to interfaces with low, medium and high interface state densities.

of disorder, E_{HO} is the trace energy per bond of the sp^3 Hamiltonian and remains invariant. In fact, it has recently been shown[6] that band line-up of an ideal heterojunction without DIGS itself is determined by line-up of E_{HO}. The role of DIGS is to form interface depletion /accumulation barriers and to pin the Fermi level or restrict its movement, both of which are characteristic of unoptimized semiconductor homo- and hetero-interfaces.

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