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IDENTIFICATION OF RESIDUAL IMPURITIES IN Si-DOPED MBE GROWN GaAs

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The changes of dopant vaporization enthalpy in GaAs:Si grown by molecular beam epitaxy revealed the presence of residual donors related to group VI elements. This has been confirmed by deep level transient spectroscopy studies of AlGaAs:Si layers grown in the same MBE system. It is argued that a commonly observed deep trap labelled E2 is probably related to Te, Se or S. The measurements have been performed on near-ideal Al Schottky barriers grown *in situ* by MBE.

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It is generally accepted that Si is an almost ideal dopant for *n*-type GaAs grown by molecular beam epitaxy (MBE). At present the layer doping is still largely empirical and often, at low doping levels residual impurities disturb calculated dependences. Usually shallow acceptors can be readily identified by low temperature photoluminescence measurements. The chemical identities of shallow donors are more difficult to determine by simple methods, and resort has to be made to far-infrared photothermal ionization or very high resolution Zeeman photoluminescence studies.

In this paper we discuss an unintentional co-doping process during the growth of GaAs:Si by MBE. Thick epitaxial layers of GaAs were grown at 580°C on semi-insulating (001) oriented GaAs using the Riber 32P MBE system, which has a background pressure $< 1 \times 10^{-10}$ torr. High purity Ga (7N), As (7N) and Si ($< 10^{12}$ cm⁻³ intrinsic) source materials were used. To achieve a full range of Si concentration the temperature of Si effusion cell was changed from 550°C to 1130°C, whereas those of Ga and As were held constant at 945°C and 218°C, respectively. The beam equivalent pressure As/Ga ratio was equal to 9.5. All layers were grown at constant rate 1 μm/h. Electrical properties of the epitaxial layers were characterised by Van der Pauw measurements. The effects of surface and

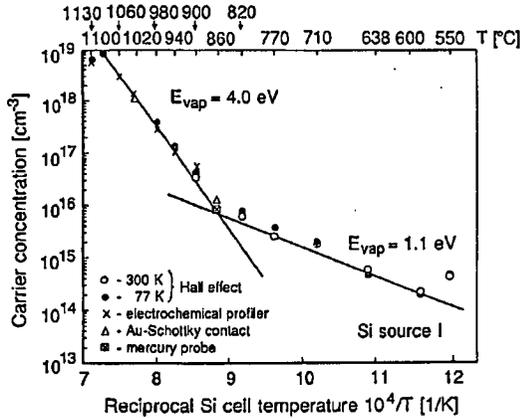


Fig. 1. Electron concentration versus reciprocal temperature of Si cell for MBE GaAs:Si with $T_{\text{sub}} = 580^\circ\text{C}$.

interface depletion layer have been taken into account. Net donor concentration at room temperature was also determined from C - V characteristics either by use of the Bio-Rad electrochemical profiler or conventional Au Schottky diodes.

Since $I_{\text{Si}} = K \exp(-E_{\text{vap}}/kT)$, where I_{Si} is the Si flux and E_{vap} is its enthalpy of vaporization, the proportionality between Si flux I_{Si} and the donor concentration can be demonstrated most readily by establishing that an exponential dependence exists between the donor concentration and the Si source temperature. This is seen in Fig. 1, from which the value of E_{vap} at a concentration higher than $1 \times 10^{16} \text{ cm}^{-3}$ is determined to be 4.0 eV, which is close to the commonly accepted value of 4.1 eV. However, at lower concentrations the enthalpy is reduced noticeably, indicating the presence of residual donors. A value determined, being equal to 1.1 eV, is close to vaporization enthalpy for VI group elements, i.e., S (0.9 eV), Se (1.0 eV) and Te (1.2 eV). It is well known that these elements exhibit the DX behaviour and can be detected in $\text{Al}_x\text{Ga}_{1-x}\text{As}$, $x > 0.2$ as deep states. In order to confirm the presence of residual donors in our growth environment deep level transient spectroscopy (DLTS) studies have been performed on special test structures.

The investigations have been carried out on near-ideal Al Schottky barriers produced by MBE on the top of the following structures: $0.5 \mu\text{m}$ n -type buffer layer doped to $2 \times 10^{18} \text{ cm}^{-3}$, 10 period GaAs-AlGaAs superlattice ($0.1 \mu\text{m}$ thick), $0.1 \mu\text{m}$ undoped graded $\text{Al}_x\text{Ga}_{1-x}\text{As}$ layer and $3 \mu\text{m}$ $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ layer doped with Si to the level $2.5 \times 10^{16} \text{ cm}^{-3}$. The superlattice was introduced to improve a quality of layers by preventing entering of extended defects into the $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ layer. After the termination of the layer growth a clear (3×1) reconstruction of As stabilised surface was observed by means of reflection high energy electron diffraction (RHEED) technique. Next the temperature of substrate was lowered to 20°C at chamber overpressure better than 4×10^{-10} torr and the Al metallic layer was deposited at pressure 5×10^{-11} torr at the rates: first $3 \text{ \AA} - 0.01 \text{ \AA/s}$ and the following $0.2 \mu\text{m} - 0.2 \mu\text{m/h}$. *Ex situ* observations of RHEED patterns and double crystal X-ray diffraction showed that the Al layer had a (001) oriented

single crystal structure. The determined [110] crystallographic direction of Al unit cell is aligned with the [100] direction in GaAs unit cell. In order to estimate the Al crystal perfection, the symmetric 002 and asymmetric 113 rocking curves were measured. The half-width (FWHM) of the 002 rocking curve was $20'$ due to a slightly mosaic structure and a small thickness ($0.2 \mu\text{m}$) of the layer.

The electrical quality of the Schottky diodes was tested by means of current-voltage (I - V) and capacitance-voltage (C - V) measurements. I - V forward characteristics, accurately exponential over 9 decades have been measured. The ideality factor $n = 1.030 \pm 0.005$ at a wide temperature range, from 275 K to 340 K, have been determined. The excellent quality of Schottky contacts allowed us to determine the barrier height φ_b from (I - V) vs. T and C - V characteristics [1]. The contributions from Γ , L and X minima have been taken into account [2]. It has been found for Al/ $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ Schottky contact $\varphi_b^{I-V} = 1.07 \text{ eV}$ and $\varphi_b^{C-V} = 1.14 \text{ eV}$. The obtained values are similar to that obtained by Missous et al. at a slightly lower Si concentration [3].

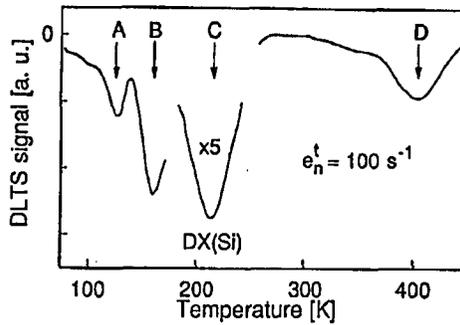


Fig. 2. DLTS spectra of $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}:\text{Si}$ MBE layers obtained at pulse duration time $50 \mu\text{s}$ and emission rate $e_n^t = 100 \text{ s}^{-1}$.

The same test structures were used for DLTS studies performed at a constant voltage as well as constant capacitance modes. A typical DLTS spectrum for majority carrier pulses is illustrated in Fig. 2. Four deep levels labelled A-D have been detected in a temperature range from 77 K to 450 K. Their thermal activation energies ΔE and concentrations N determined from emission characteristics are as follows: $\Delta E^A = (0.21 \pm 0.02) \text{ eV}$, $N^A = 4 \times 10^{13} \text{ cm}^{-3}$, $\Delta E^B = (0.26 \pm 0.02) \text{ eV}$, $\Delta E^C = (0.42 \pm 0.02) \text{ eV}$, $\Delta E^D = (0.79 \pm 0.01) \text{ eV}$, $N^D = 3 \times 10^{13} \text{ cm}^{-3}$. The energies of states A and B were determined at low emission rates, when they were well separated from the trap C. The dominant trap C is clearly related to the well-known DX (Si). The trap D observed at a low concentration has been identified as E6 which is related to a complex associated with Ga vacancy and an oxygen atom [4] or an Al-O complex [5]. The traps A and B well fit to unidentified levels labelled E1 and E2 that were often observed in AlGaAs grown by MBE [6]. On the other hand the trap B fits with high accuracy to the level related to DX (Te) ($\Delta E = 0.27 \text{ eV}$), studied by Dobaczewski et al. [7]. However, its relation to S or

Se is also possible since the thermal activation energy ($\Delta E \approx 0.28$ eV) as well as the DLTS peak position are the same for all group VI elements [8].

The measurements of DLTS peak height vs. pulse duration time t_c for all the traps studied have also been performed. It has been found that the peak height of the traps *A* (E1) and *D* (E6) were almost unchanged when t_c was reduced to 1 μ s, showing a high value of capture cross sections of these states. In contrast to that, the peak height of traps *B* and *C* (DX(Si)) were significantly reduced at short pulses.

The results obtained from DLTS studies for level *B* and the determined value of vaporization enthalpy suggest that this trap is related to the group VI element. It should be noticed that in such a case a concentration of the trap determined from DLTS is underestimated due to its DX character. The correspondence of the trap *B* to the level E2 indicates a common MBE problem of the presence of traces of these impurities in the growth environment.

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