Electron Traps in GaAs Grown by Molecular Beam Epitaxy on On-axis (100) and Off-axis Substrates

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ABSTRACT

Deep level transient spectroscopy (DLTS) was used to characterize the electron traps present in the bulk GaAs grown by molecular beam epitaxy (MBE) on on-axis (100) and off-axis (4° towards the (111) A direction) substrates. Two electron traps were obtained for each sample having identical corresponding peak locations in the DLTS spectra. The layer grown on the on-axis substrate has electron traps with activation energies of E_c -0.454 eV and E_c -0.643 eV and capture cross-sections of 1.205 x 10⁻¹⁴ cm² and 3.88 x 10⁻¹⁵ cm², respectively. The layer grown on the off-axis substrate has traps with activation energies of E_c -0.723 eV and capture cross-sections of 2.060 x 10⁻¹⁴ cm² and 4.40 x 10⁻¹⁴ cm². The electron traps are possibly the M4 (or EL3) and EL2 (or EB4) traps commonly found in GaAs layers. Due to the high trap concentrations obtained and to the non-uniform trap concentration profile, As desorption may be considerable during growth.

INTRODUCTION

Molecular beam epitaxial (MBE) growth of GaAs started in the 1970s and film characterizations such as x-ray diffraction, hall measurements, and various optical methods have since followed to determine the quality of the grown layers. Another very useful technique for layer quality evaluation is deep level transient spectroscopy (DLTS) (Lang, 1974) first developed by Lang et al. As defects in the crystal structure may form deep levels in the forbidden gap, DLTS could be used to measure the activation energy and apparent capture cross-section of carrier traps. It could also determine the concentrations of the traps in the semiconductor.

MBE-grown GaAs was found to have nine different traps labeled M0 to M8 depending on the growth conditions used (Farrow, 1995; Blood & Harris, 1984). Traps M1, M3, and M4 occur reproducibly for n-GaAs grown under the (2x4) Asrich conditions (Xu et al., 1987; Blood & Harris, 1984; Gombia et al., 1994).

It has also been found that optical, electron transport, and morphological epilayer properties were highly improved when (100) GaAs substrates misoriented by a few degrees toward the (111) A direction were used (Blood & Harris, 1984; Radulescu et al., 1987).

It is the intent of this work to compare traps found in the GaAs layers grown on an on-axis (100) substrate and on an off-axis substrate.

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THEORY

A reverse bias varies the width of the space-charge region in a metal n-type semiconductor schottky contact so that its capacitance changes. If deep levels are present, traps can be depleted and filled with electrons of different amounts of reverse bias applied. The very small change in capacitance (transient) due to the filling and emission of electrons from the trap sites is detected. Assuming that the traps are initially filled, its emission rate then is (Schroder, 1990):

$$e_n / T^2 = \gamma_n \sigma_n exp \left[-\frac{E_c - E_T}{kT} \right]$$
(1)

where *T* is the absolute temperature, k is the Boltzmann's constant, E_c is the conduction band edge, E_T is the trap level, and σ_n is the apparent capture cross-section of the trap. The parameter $\gamma_n = (v_{th} / T^{1/2})(N_C / T^{3/2})$ where v_{th} is the thermal velocity of electrons and N_c is the effective density of states in the conduction band.

The emission rate is the inverse of the time constant, τ_e , of the capacitance transient which, in turn, is known to obey the relation (Schroder, 1990):

$$C = C_o \left[1 - \frac{n_T(0)}{2N_D} \exp\left(-\frac{t}{\tau_e}\right) \right]$$
(2)

where C_0 is the capacitance at the original reverse bias, $n_T(0)$ is the original number of electrons per unit volume occupying the trap level during the transient, N_D is the doping concentration, and t is the time. Hence, if the doping concentration is known, $n_T(0)$ can be obtained. For a sufficient filling pulse, this can be taken as the trap concentration N_T .

The activation energy $E_{act} = E_C - E_T$, and capture crosssection σ_n along with the trap concentration N_T and temperature peak location in the DLTS spectrum comprise the signature of the particular trap present in the semiconductor.

EXPERIMENTAL METHOD

One and a half micron $(1.5 \ \mu\text{m})$ GaAs was grown by MBE on the on-axis and off-axis substrate simultaneously in order to have identical growth

conditions. The films were doped with Si to obtain doping concentrations of around 10^{17} cm⁻³. A typical growth temperature of around 630°C and beam fluxes of the As₄ and Ga that would give a (2x4) surface reconstruction were utilized. Schottky barrier diodes (SBDs) were made out of the samples by deposition of 1 mm-diameter aluminum dot Schottky contacts on the top layer and indium as backside ohmic contact.

After obtaining the doping concentrations, DLTS characterization was performed on the two samples using a DLS-83D apparatus made by Semilab, Hungary. Different excitation frequencies were used for temperature scans of 77 K to 400 K each. This makes the DLTS signal (proportional to the change in capacitance and, therefore, to the emission rate) peak at different temperatures. An emission rate-temperature data pair could then be obtained. From Eq. (1), necessary trap parameters E_{act} and σ_n could be calculated. The height of the DLTS peak is related to N_T from Eq. (2).

Depth profiling of the deep level was obtained by choosing a frequency-temperature data pair, which belongs to the given deep level. By using two reverse bias pulses of different heights, the depth region could be selected. These two pulses would be changed step by step while the difference of the pulse heights was kept constant during the measurement.

The DLTS signal coming from the selected deep level would, thus, be plotted as a function of depth.

RESULTS AND DISCUSSION

The DLTS spectra for the samples grown on the onaxis substrate (L047-on) and on the off-axis substrate (L047-off) are shown in Fig. 1. A peak is assumed to be due to one kind of trap. The emission ratetemperature data pair for each peak can be plotted in an $\ln(e_n/T^2)$ vs 1/T axis called an Arrhenius plot. Those of peaks P1 are shown in Fig. 2 where least-square lines were fitted. From Eq. (1), it can be shown that the slope of the line is E_{acl}/k and the y-intercept is just $\ln(\gamma_n \sigma_n)$. Table 1 shows the obtained trap parameters along with the possible identities of the traps based from the work of others. Finally, Fig. 3 shows the depth profiles for trap P1 for L047-on. That for L047-off is very similar.



Fig. 1. DLTS Spectra of (a) L047-on and (b) L047-off at frequencies: (i) 2500 Hz; (ii) 250 Hz; (iii) 25 Hz; and (iv) 2.5 Hz. A quiescent reverse bias/ filling pulse of -3V/-1V was used for all the measurements. Excitation pulse widths were varied.



Fig. 2. Arrhenius plots for P1 in the DLTS spectra for (a) L047-on and (b) L047-off at frequencies (i) 2500 Hz; (ii) 250 Hz; (iii) 25 Hz; and (iv) 2.5 Hz.

It can be seen in Table 1 that there is not much difference between the trap parameters of P1 for L047-on and L047-off. Due to the difficulty of resolving the Arrhenius plots for P2, the E_{act} and σ_n , data shown in Table 1 are obtained from DLTS measurements of the substrates as the second deep level was observed to be present also in the substrates. The P2 data for L047-off are more accurate since there were 3 scans (not shown

Sample	Trap Label	Peak Location (K)⁺	Activation Energy, <i>E_{act}</i> (eV)	Capture Cross- section, σ_n (cm ²)	Trap Concentration, <i>Ν_τ</i> (cm ⁻³)	Possible Trap Identity
L047-on	P1	272.1	0.454 ± 0.001	$(1.205\pm0.035) \times 10^{-14}$	4.37 x 10 ¹⁶	EL3, M4
	P2	382.8	0.643 ± 0.028	$(3.88\pm2.55) \times 10^{-15}$	1.70 x 10 ¹⁶	EL2, EB4
L047-off	P1	265.1	0.514 <u>+</u> 0.006	(2.060±0.560) x 10 ⁻¹⁴	1.97 x 10 ¹⁷	EL3, M4
	P2	382.1	0.723 <u>+</u> 0.010	(4.40±1.47) x 10 ⁻¹⁴	5.15 x 10 ¹⁶	EL2, EB4

Table 1. Trap parameters for the deep levels of L047-on and L047-off and their possible identities.

⁺Peak temperature measured at a scan of 250 Hz.



Fig. 3. Depth profile of electron trap P1 for L047-on.

here) performed. Due to the closeness of the peaks P1 and P2 for the on- and off-axis samples, the corresponding traps were assumed to be of the same chemical origin. The first electron trap with a lower temperature peak corresponds to either the trap M4 (Blood & Harris, 1977) found in MBE-grown GaAs or the trap EL3 (Martin et al., 1977) commonly found in LPE-grown samples. M4 was identified to be an impurity-related trap involving As vacancies (Blood & Harris, 1984). If this is the trap observed, then some mechanism must have been desorbing much of the As atoms during growth. This might explain the high rap concentrations obtained which were only an order of magnitude lower than the doping concentrations. The substrate temperature might not be accurate since the thermocouple is behind the molybdenum block substrate holder. This is supported by the non-uniform distribution of this trap as seen in Fig. 3.

The second electron trap observed is either the trap EL2 (Martin et al., 1977) or EB4. If it is EL2, which is an As antisite-related (AsGa-X) trap, then this explains the earlier depletion of As. Some of the As atoms that did not desorb from the grown layers might have replaced some of the Ga atoms in the lattice.

CONCLUSIONS

At the growth conditions used, there seems to be no difference in trap incorporation in GaAs films grown on on-axis (100) and off-axis (tilted 4° towards the (111)A direction) substrates. Two traps are present in the bulk samples possibly corresponding to M4 or EL3 and EL2 or EB4, respectively. As M4 is an impurity-related trap involving As vacancies, the growth temperature might be higher than expected and As desorption are not uncommon. It is likely that a fraction of As atoms that produced the vacancies occupied Ga sites in the lattice producing the EL2 defect.

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