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Atomic layer epitaxial predeposition for GaAs growth on Si

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We report a two-step growth process, using an atomic layer epitaxially grown GaAs predeposition layer for the growth of GaAs/Si layers by metalorganic vapor phase epitaxy technique. Photoluminescence and deep-level transient spectroscopy techniques are used to show that the quality of the grown material is comparable to that grown by a much complicated procedure involving strained layer superlattice buffers introduced between the active GaAs layer and the Si substrate. © *1996 American Institute of Physics.* [S0003-6951(96)01225-9]

Heteroepitaxial growth of III–V semiconductors on Si substrates is an important emerging technology with potential applications in integration of Si electronic devices with III–V electro-optic devices. GaAs epitaxy on Si has received the most attention. However, the large lattice mismatch at the heterointerface and the difference in thermal expansion coefficients between GaAs and Si induce a high density of dislocations and residual stress in GaAs layers. The nonpolar/polar character of the two semiconductors gives rise to antiphase domain (APD) formed by As–As or Ga–Ga bonds.[1] Insertion of strained-layer superlattice (SLS)[2] has been used to reduce threading dislocations. Several other techniques such as low-temperature growth,[3] mechanical compensation of the size difference between GaAs and Si,[4] mesa edge stress release,[5] undercut GaAs (UCGAS),[6] and post-growth annealing[7] have been used to reduce thermal stress and dislocation density. Most of these involve either complicated growth procedures or post-growth processing although they all adhere to the well-established two-step growth scheme.[8] Poor performance of devices fabricated on GaAs/Si may be attributed to APDs which make the epitaxial layer behave like a highly compensated semiconductor. Two-dimensional (2D) growth, instead of three-dimensional island-type growth, favors reduced density of APDs.[9] Kitahara *et al.*[10] showed that, in the case of GaAs growth by atomic layer epitaxy (ALE), 2D growth started at an early stage. In this letter, we propose a two-step growth scheme where the initial predeposition stage is performed by ALE in an atmospheric pressure metalorganic chemical vapor deposition (MOCVD) system. The luminescence and deep-level properties of the grown material are studied and compared with that of layers grown both by conventional two-step technique and with SLS buffers introduced.

The (100) Si substrates used for growth were *n* type with carrier concentrations greater than 1×10^{18} cm^{-3}. The substrates were 2×1 cm^2 in area and 3° miscut toward ⟨110⟩. Substrate cleaning was done in organic solvents followed by oxide removal in buffered HF etchant. Finally, the surface of the substrate was hydrogen terminated using a 1:1 HF:H_2O dip and spun dry under flowing nitrogen. The samples were quickly introduced into the load-lock chamber and then baked under arsine/hydrogen ambient at 970 °C.

In the first run (sample I), a two-step growth process was employed in which a 20-nm-thick GaAs layer was predeposited at 425 °C, followed by 725 °C anneal for 10 min. Subsequently a 2 μm epitaxial layer was grown at an optimized temperature of 650 °C at the growth rate of 1.5 μm/h. Two modifications were next introduced in the predeposition layer. First, a 10-period (2 nm) $GaAs_{0.91}P_{0.09}$/(2 nm) GaAs SLS was grown at 650 °C before the growth of the top 2 μm GaAs layer (sample II). The thickness of $GaAs_{0.91}P_{0.09}$ was within the critical thickness, and the strain component was kept low to avoid a rough surface.[11] Second, the 20 nm predeposition layer was grown using ALE (sample III) and the 725 °C anneal was eliminated. The Ga and As sources were switched alternatively to the reactor for periods of 3 s with 1 s intervals. The As flow rate was switched between 80 and 5 sccm. The flow rates of trimethylgallium (TMG) and AsH_3 were maintained to obtain a growth rate of 400 nm/h for GaAs/GaAs. A 5 sccm flow rate during As off-period was maintained to prevent As evaporation, unlike that of Lee *et al.*[12] where the growth was more like migration-enhanced epitaxy (MEE).

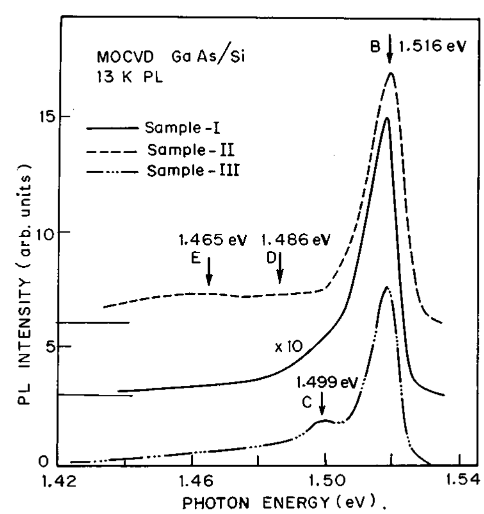

FIG. 1. PL spectra for GaAs/Si samples grown under three different conditions.

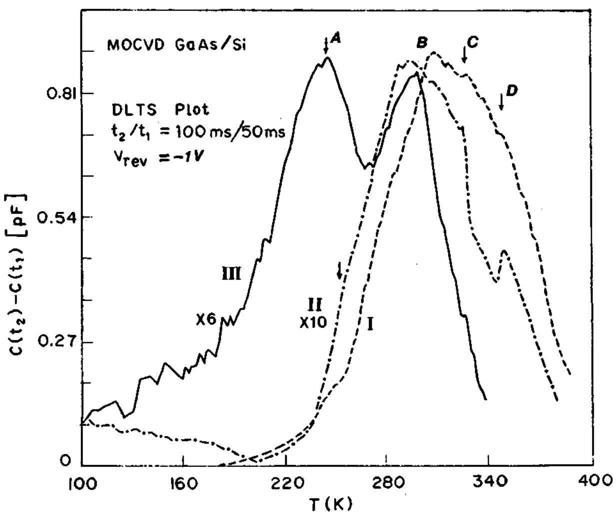

FIG. 2. DLTS spectra for electron traps in samples I, II, and III.

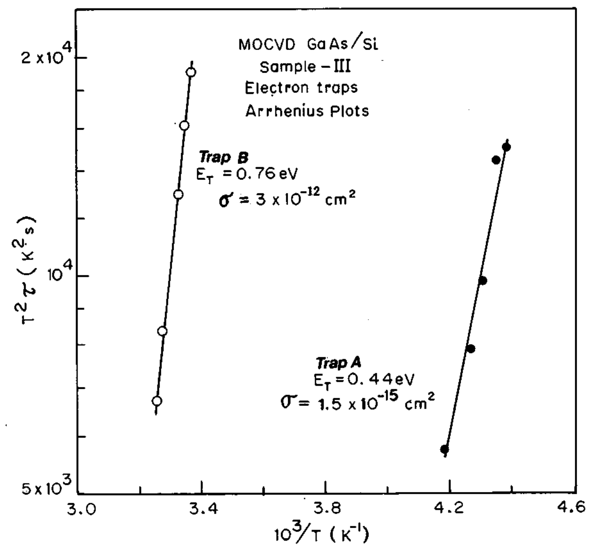

FIG. 3. Arrhenius plots for electron traps A and B.

The undoped layers were *n* type with free-electron concentrations around 10^{17} cm^{-3}. This value is about two orders higher than that for GaAs/GaAs layers grown under similar conditions and can be attributed to substrate autodoping effects.[11]

The epitaxial films were characterized by 13 K photoluminescence (PL) and deep-level transient spectroscopy (DLTS). PL excitation was obtained from the 514.5 nm line of an argon ion laser and the luminescence spectra were detected with a 0.64 m spectrometer and S1 photomultiplier. The excitation level was kept constant at 0.4 kW/cm^2. The PL spectra of samples I, II, and III are shown in Fig. 1. The spectra are dominated by a peak ''B'' at 1.15163 eV arising from the conduction-band-to-carbon acceptor and donor-to-carbon acceptor. It is interesting to note that, for the excitation power varying from 0.28 to 11.5 kW/cm^2, the peak energy shift is <1 meV. This indicates low incorporation of defects. The absence of splitting of the light- and the heavy-hole transitions, unlike Ref. 12, shows the absence of any substantial strain developed in the epitaxial layer during cooling. The full width at half maxima (FWHM) are 13.8, 12, and 12.4 meV for samples I, II, and III, respectively. The values of FWHM are almost double that of GaAs/GaAs grown under identical conditions and are similar to those observed by others at similar excitation levels.[11] The peak intensity increases by an order of magnitude in sample II compared to sample I, but shows the emergence of the familiar ''D'' and ''E'' peaks, which are known to occur due to extraneous impurity related sources.[1] A reduction of peak intensity by about 35% is observed in sample III compared to sample II with the notable absence of the D and E peaks. A peak ''C'' appears at 1.499 eV, which is 20 meV below the dominant B peak indicating the presence of residual carbon impurities.[13] The relative integrated intensities of luminescence are 0.13, 1.67, and 1.00 for samples I, II, and III, respectively.

DLTS measurements were done on evaporated gold Schottky barrier diodes (0.5 mm diameter) fabricated on the cleaned surface of the layer. The description of our DLTS system is given elsewhere.[14] Figure 2 shows the DLTS spectra of electron traps, detected in samples I, II, and III. Each spectrum is characterized by a prominent peak at 300–310 K, corresponding to an electron trap B. Sample III, in addition, contains a second peak, equal in magnitude to that for B, which we associate with another electron trap A. Presence of this trap is also indicated in the other two samples as weak shoulders. On the high-temperature side, we note shoulders due to two more electron traps which we label as traps C and D. The observed DLTS spectra, in particular that for sample III, are similar to the one obtained by Soga *et al.*[15] in GaAs/Si grown by MOCVD with GaP/$GaAs_{0.5}P_{0.5}$ and $GaAs_{0.5}P_{0.5}$/GaAs SLS buffers. The sharp DLTS peaks for traps A and B, obtained in sample III, are used to get their Arrhenius plots which are presented in Fig. 3. It is apparent that traps A and B are the same as the 0.44 and 0.73 eV electron traps detected by Soga *et al.* in their materials. From the variation of the trap density with GaAs thickness, these authors inferred that the 0.73 eV trap is probably EL2 and the 0.44 eV trap is related to Si defect complexes arising out of Si, autodoped into the epitaxial layer. From published data,[16] however, we observe that trap B is more likely to be identified with EL12, previously found in vapor phase epitaxial GaAs. On the other hand, the temperature position of trap D in our data for samples I and II suggests that it is perhaps due to EL2 with trap C as one of its associate family members. If so, this observation suggests that EL2 is either absent or present in much lower density in sample III, compared to that in samples I and II.

Finally, the densities of the electron traps in samples I, II, and III are measured from DLTS peak heights and from the approximate positions of the shoulders. These values are presented in Table I. It is evident that both ALE predeposition and SLS buffering drastically reduce the density of traps

TABLE I. Trap densities in GaAs/Si layers.

Sample No.	Density (cm^{-3}) of			
	Trap A	Trap B	Trap C	Trap D
I	2.8×10^{15}	1.6×10^{16}	1.4×10^{16}	1.2×10^{16}
II	7.3×10^{14}	1.4×10^{15}	1.2×10^{15}	8.0×10^{14}
II	2.8×10^{15}	2.7×10^{15}	⋯	⋯

B, C, and D and, in comparison with PL results, we can say that these are the main radiation killers in GaAs/Si. We also note that traps D, which are likely EL2 traps, are not detected in sample III which is a positive feature of our proposed growth technique. The density of trap A, believed to be due to Si defect complexes, is almost equal in samples I and III but much lower in sample II, grown with a SLS buffer.

In summary, we have proposed a MOCVD growth technique for GaAs/Si where the initial predeposition step is done by ALE to obtain layers with good optical quality and dramatically reduced density of two deep traps (C and D) while maintaining the density of deep traps A and B comparable to the other current growth procedures. A key feature of this technique is the elimination of complicated growth sequence as in the case of growth with SLS buffers. The observed traps in the material are identified with known traps previously observed in MOCVD GaAs/Si and in VPE GaAs.

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