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Studies on deep levels in GaAs epilayers grown on Si by metal–organic chemical vapour deposition
Part IV: 0.96 eV photoluminescence emission

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Much attention has been paid to the growth of heteroepilayers on Si. Recently the electrical and optical properties of GaAs epilayers grown on Si substrates (GaAs/Si) have been studied extensively because of their potential applications for optoelectronics [1–4].

In this work, we studied the temperature and excitation intensity dependent near-infrared photoluminescence (NIPL) related to the deep levels present in GaAs/Si by metal–organic chemical vapour deposition (MOCVD). Taking into account the Frank–Condon (FC) and bandgap shifts, we reformulated the energy relationship for the recombination luminescence of donor–acceptor pair (DAP) and proposed that the 0.96 eV emission could be interpreted as the recombination luminescence of the DAP, composed of an arsenic vacancy donor V_{As} and a gallium vacancy acceptor V_{Ga}.

The 1.2 μm thick GaAs epilayers used for the experiments were grown by MOCVD on the *n*-type (1 0 0) Si substrates misorientated 4 towards one of the (1 1 0) directions using the two-step method [1]. The Si substrates were chemically treated in NH_4OH, H_2O_2, H_2O and HCl, H_2O_2, H_2O, and etched in HF for 1 min. In H_2/AsH_3 ambient, they were heated initially at 1000 °C for 10 min, and the temperature was lowered to 400–450 °C for GaAs buffer growth with thickness of 25 nm. Trimethylgallium (TMG) and arsine in hydrogen were used as source chemicals. Then, the temperature was raised to 700 °C, and the top GaAs epilayers were grown with the ratio of [As]/[Ga] $\simeq$ 20 and with a growth rate of 100 nm min^{-1}. The samples were not intentionally doped. The carrier concentration at room temperature was $\sim 2 \times 10^{17}$ cm^{-3}.

The temperature and excitation intensity dependent NIPL spectra of GaAs/Si epilayers were obtained with an ordinary gating monochromator and were detected by a liquid nitrogen-cooled Ge detector using a conventional lock-in technique. Luminescence was excited with the 632.8 nm line of an He–Ne laser. The measured temperature was 77–300 K and the excitation intensity was 10^{-2}–10^{2} W cm^{-2}.

Fig. 1 shows the NIPL spectrum of the GaAs/Si epilayer at 77 K and the excitation intensity 1.0 W cm^{-2}. The spectrum can be fitted by a sum of two Gauss-type curves including a main peak 0.96 eV and a shoulder 0.84 eV. The discrepancy between experimental points and Gauss-type curves at the right tail, as shown in Fig. 1, arises from the existence of another weak peak with energy 1.13 eV, which we have explained as the recombination luminescence of DAP, composed of an Si shallow donor on the Ga site and a Ga vacancy acceptor [5].

The temperature dependent PL spectra of the GaAs/Si epilayer were carried out in the temperature range 77–300 K. As shown in Fig. 2, with the increase of temperature, the full width at half maximum (FWHM) of the 0.96 eV emission band increased and the peaks position changed by no more than 0.005 eV.

Fig. 3 shows the variation of PL intensity with

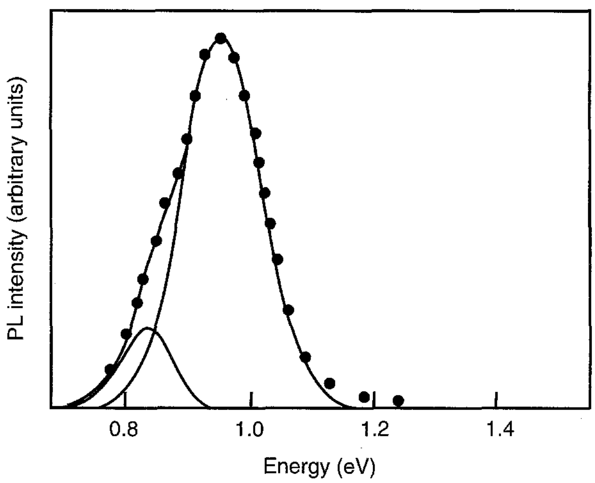

Figure 1 NIPL spectrum of the GaAs/Si epilayer at 77 K and excitation intensity 1.0 W cm^{-2}. (●), Experimental points.

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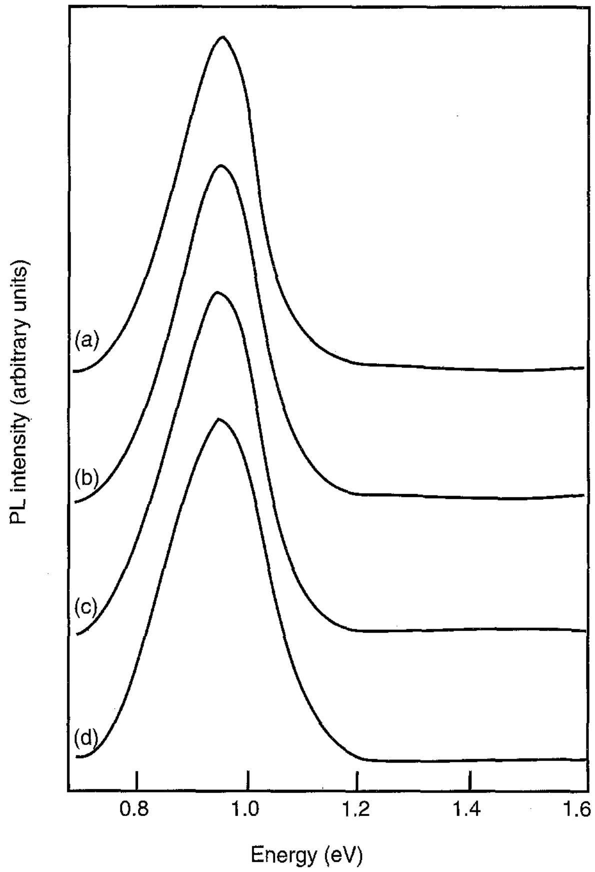

Figure 2 NIPL spectra of the GaAs/Si at (a) 77 K, (b) 110 K, (c) 186 K and (d) 250 K.

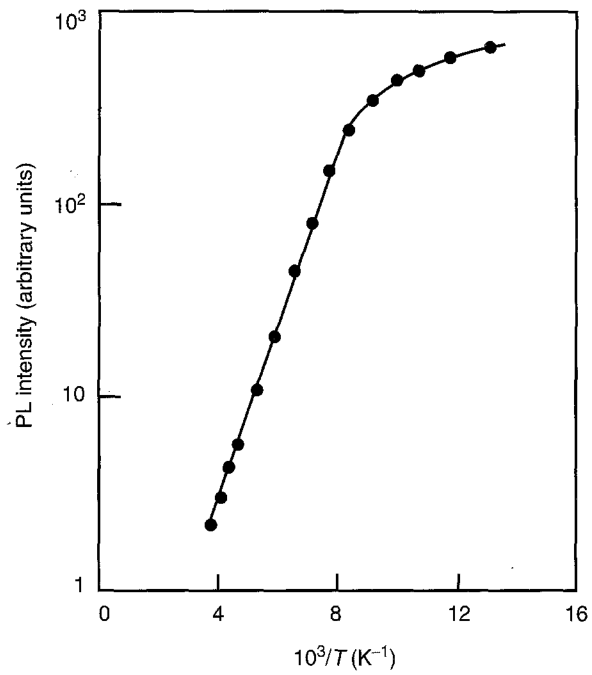

Figure 3 Temperature dependence of PL intensity for 0.96 eV emission.

temperature for the 0.96 eV emission. In terms of experimental data, the thermal activation $\Delta E = 0.10$ eV for the 0.96 eV emission was obtained by using an Arrhenius plot:

$$I = C \exp(\Delta E/kT). \quad (1)$$

where I is the PL intensity and C a constant.

Fig. 4 shows the variation of the FWHM of the 0.96 eV emission in the GaAs epilayer with the square root of temperature. According to the configurational coordinate model [6], the theoretical temperature dependence of FWHM $W(T)$ can be expressed by:

$$W(T) = (8 \ln 2)^{1/2} S^{1/2} \hbar\omega [\coth(\hbar\omega/2kT)]^{1/2} \quad (2)$$

where S is the Huang–Rhys constant, and $\hbar\omega$ is the phonon energy. The solid line in Fig. 4 is the fit of Equation 2 to experimental data with $\hbar\omega = 36$ meV and $S = 3.2$. The Huang–Rhys factor $S > 1$ indicates that there exists a strong electron-lattice coupling, which leads to the 0.96 eV emission band having a broad Gaussian lineshape without any fine structure [5–7]. Thus, the FC shift Δ_{FC} is given by $\Delta_{FC} = S\hbar\omega = 0.11$ eV.

Kim *et al.* [8] established a relation of bandgap shift to temperature in GaAs. Liang *et al.* [9] indicated that taking into account the FC and bandgap shifts, the energy relationship of DAP recombination luminescence could be reformulated as:

$$\hbar\omega = (E_g)_{max} - \Delta E_g - (E_d + E_a - e^2/\varepsilon r) - \Delta_{FC} \quad (3)$$

where $\hbar\omega$ is an emission peak energy, E_a and E_d are the binding energies of isolated donor and acceptor, respectively, $-e^2/\varepsilon r$ is the Coulomb interaction energy of DAP, $(E_g)_{max}$ is the maximum of the bandgap and ΔE_g is the shift of bandgap. For GaAs, $(E_g)_{max} = 1.517$ eV and:

$$\Delta E_g = aT^2(b + T) \quad (4)$$

where T is the measured temperature of epilayers (in K), $a = 5.6 \times 10^{-4}$ eV K^{-1} and $b = 226$ K [8].

Experiments [10–12] indicated that in GaAs Ga vacancies V_{Ga} always exist at ~0.3 eV above the valence band. Besides, our experiments demonstrated that with the increase of the ratio of [As]/

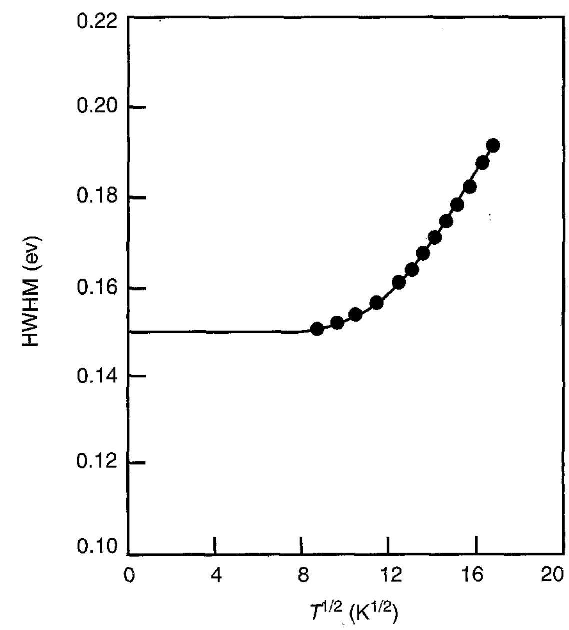

Figure 4 Variations in FWHM with $T^{1/2}$ for 0.96 eV emission.

[Ga], which reduces the concentration of the As vacancy V_{As} in GaAs, the PL intensity of the 0.96 eV emission rapidly decreases. This means that the 0.96 eV emission possibly depends on the V_{As}. Ambigapathy *et al.* [13] investigated the ionization energies of V_{As} in GaAs and found that one of them is located at 140 meV, below the bottom of the conduction band. The V_{As} and V_{Ga} in question comprise the DAP. Both theoretical and experimental values of the deep levels of V_{As} and V_{Ga} are in good agreement [10–14]. According to Equation 3 and these experimental data, the transition energy of the DAP, composed of V_{As} donor and V_{Ga} acceptor, is equal to ~0.96 eV, which is in good agreement with our experiments as shown in Fig. 1.

Harrison *et al.* [15] interpreted the 0.99 eV emission in Si-doped GaAs grown by molecular beam epitaxy on (1 0 0)-orientated substrates as transition of the pair Si_{Ga}–Si_{As}, composed of Si on Ga site and on As site, respectively. Experiments indicated that donor Si_{Ga} and acceptor Si_{As} are at 5 meV below the bottom of the conductor band [11] and at 35 meV above the top of the valence band [16] in GaAs, respectively. In fact, the transition energy of the Si_{Ga}–Si_{As} pair should be much higher than 0.99 eV, so 0.96 eV emission might originate from the transition of V_{As}–V_{Ga} pair instead of Si_{Ga}–Si_{As} pair.

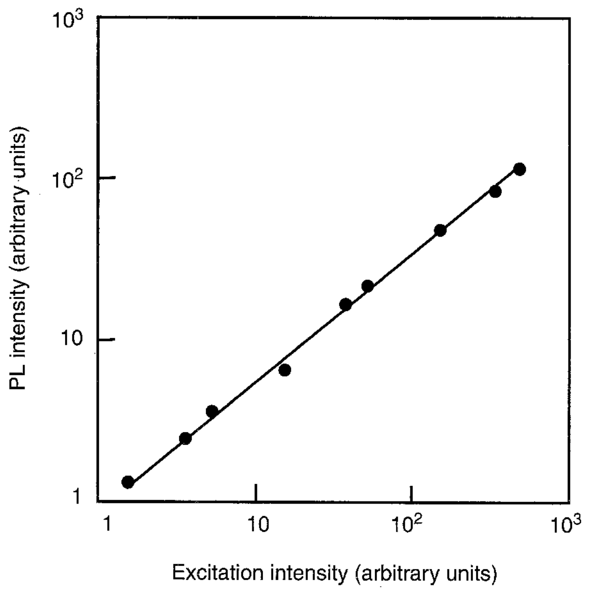

Figure 5 Excitation intensity dependence of PL intensity for 0.96 eV emission at 77 K.

The dependence of the PL intensity on excitation intensity for 0.96 eV emission at 77 K is shown in Fig. 5, which can be expressed as:

$$I_{PL} = KI_{ex}{}^{n} \quad (5)$$

where I_{PL} is the measured PL intensity, I_{ex} the excitation intensity, K a proportional constant and $n = 0.79$. It means that there exist non-radiative traps in GaAs/Si for $n < 1$.

Acknowledgements

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