

Band-Gap Narrowing in Carbon Doped GaAs with Various Substrate Orientations Studied by Photoluminescence Spectroscopy

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1. Introduction

The effects of carbon doping on GaAs are of importance in understanding the band-gap narrowing effect as well as for developing optoelectronic devices such as heterojunction bipolar transistors (HBT), MODFETs, and semiconductor lasers [1]. The use of carbon (C) as a p-type dopant in GaAs, AlGaAs, and InGaAs has several advantages because the heavy doping to a level as high as 10^{21} cm^{-3} is easily obtained by the property of its low diffusivity and memory effect. It is well known that with increasing carbon doping concentration, the impurity band merges with the valence band edge and generates the density of states at the band tail extending into the band gap. As a consequence, the energy band structure of GaAs epilayers is varied. Since Shaw [2] proposed that the growth rate significantly depends on the crystallographic orientation for GaAs, much efforts have made on the substrate orientation dependence of impurity incorporation and various device structures. Such devices grown on GaAs substrates with various orientations may provide innovative performance such as lateral p-n junction and lateral growth rate enhancement which can not be obtained using planar substrates.

Recently several authors have given conflicting empirical relations of the effective band-gap narrowing for C-doped GaAs as a function of hole concentration. Some of experiments support the Jain and Roulson's theory [3] while other experiments follow the Sernelius's theory [4]. In this work, we present a systematic study of the band-gap narrowing effect as a function of substrate orientation, temperature, and hole concentration in C-doped GaAs epilayers grown on GaAs (100) substrate and (n11)A substrates with $n=1, 2, 3,$ and 5 .

2. Experiments

All C-doped GaAs epilayers used in these experiments were grown on semi-insulating GaAs substrates with various crystallographic orientations by the atmospheric pressure metalorganic chemical vapor deposition in a vertical quartz reactor. The orientation of the substrates declined from (100) toward (111)A; (100), (511)A, (311)A, (211)A and (111)A. Trimethylgallium was used as the Ga precursor, AsH_3 (20 % diluted in pure hydrogen) as the As precursor, and CBr_4 as the C source. Palladium diffused hydrogen was

used as a carrier gas. The total flow rate was about 5 standard litres per minutes. The substrate temperature was set at 550°C and the ratio of V/III was kept at 60. The thickness of the epitaxial layers was measured by scanning electron microscope while the free-hole concentration was determined by the van der Pauw-Hall method. The PL measurements were carried out in a temperature range of 17 to 280 K. The photoexcitation was provided by the 514.5 nm line of an Argon ion laser. The luminescence was dispersed through a monochromator (SPEX 1702, $f=75 \text{ cm}$), and detected with a photomultiplier tube and photon counting system.

3. Results and Discussion

Figure 1 shows the PL spectra of C-doped GaAs as a function of substrate orientation at 17 K. The PL peak energy of C-doped epilayers shows a strong dependence on substrate orientation. For C-doped GaAs epilayer on (100) substrate, the PL peak position occurs at 1.456 eV. As the offset angle of substrate is increased, the PL peak position moves to higher energy of 1.490 eV at (311)A, and 1.493 eV at (211)A substrate, respectively. The blueshifts in PL peak of (211)A substrate with respect to that of (100) can be explained by the increase in PL peak energy as a result of the high desorption rate of carbon-containing species due to the lower covalent bonding strength at (211)A. For the case of impurity doped compound semiconductors, the exact

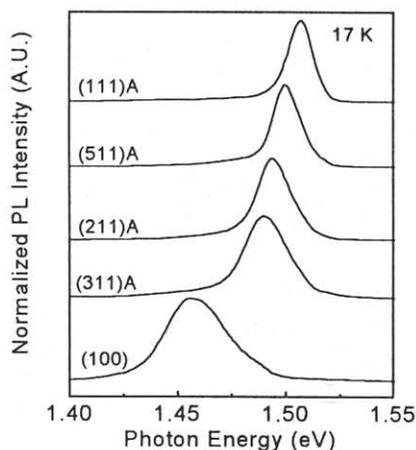


Fig. 1. PL spectra of (100), (311)A, (211)A, (511)A, and (111)A samples at 17 K.

s	p	parameters			
		α	β	E_0	dE/dT
(100)	4.5×10^{19}	4.1×10^{-4}	250	1.433	-0.245
(511)A	6.5×10^{18}	6.8×10^{-4}	250	1.470	-0.389
(311)A	3.3×10^{19}	5.1×10^{-4}	250	1.453	-0.314
(211)A	8.8×10^{18}	6.4×10^{-4}	250	1.462	-0.367
(111)A	4.6×10^{18}	7.4×10^{-4}	250	1.477	-0.403

Table I. Parameters p (hole concentration), dE/dT (temperature coefficient), and $E(0)$, α and β of Varshni equation for various substrates.

band-gap has not been well defined from an optical spectrum due to the formation of the band tails into the band gap [1]. The effective band-gap is thus determined from the intersection between the tangent to the low energy tail of the emission band and the background. Table I shows values of the parameters $E(0)$, α and β measured in the temperature range of 17 K to 280 K using Varshni equation,

$$E(T) = E(0) - \alpha T^2 / (\beta + T) \quad (1)$$

where $E(T)$ is the band-gap energy at T , $E(0)$ is the band-gap energy at zero temperature. Here the parameters α and β are determined by fitting the experimental data with Eq. (1).

Figure 2 shows the PL spectra of C-doped GaAs as a function of temperature for (100) sample. At 17 K the luminescence spectrum shows a strong emission peaking at 1.456 eV with the FWHM of 33 meV. The line has been attributed to a band to band transition. Large redshifts in PL peak energy of C-doped GaAs with increasing temperature are observed. In addition, an increase in temperature caused a gradual increase in the FWHM and developed a shoulder on the high energy side of the main emission line. The shoulder, which originates from the GaAs substrate, begins to appear at 120 K and is completely separated from the band to band emission line at 180 K. The separation of two PL peaks is measured to be 30 meV at 190 K. The observed high energy tail is probably due to a coupling of hot electron recombination with a large distribution of holes in the valence band. In order to investigate the effect of the change in temperature on the band-gap energy of C-doped GaAs, a least-square fit to the experimental data was taken. The temperature coefficient was measured to be -0.245 meV/K. Figure 3 shows the band gap narrowing of C-doped GaAs (■) as a function of hole concentration. For comparison the data of Lee et al (∇) [5], and Yan et al (\triangle) [6] are included. The band-gap narrowing with hole concentration p can be represented by

$$\Delta E_g \equiv E_g(\text{doped}) - E_g(\text{pure}) = -A p^{1/3}, \quad (2)$$

where E_g in eV, p in cm^{-3} , and A is a fitting parameter. A best fit to the experimental points (solid line in Fig. 3) gives $\Delta E_g = -2.5 \times 10^{-8} p^{1/3}$. The dashed line is a fit of Eq. (2) with $A = 2.17 \times 10^{-8}$ determined by Kim et al. [7] while the

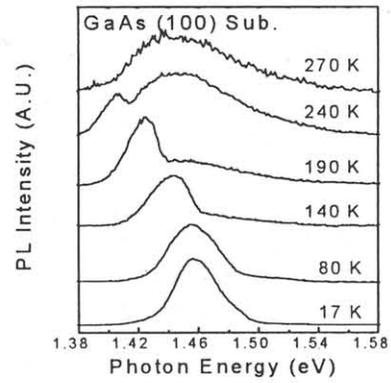


Fig. 2. Normalized PL spectra of (100) sample.

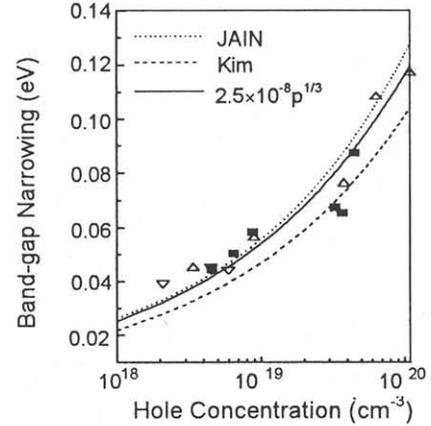


Fig. 3. Comparison of the band-gap narrowing derived from PL spectroscopy with other results.

dot line is a plot using Jain theory.

4. Conclusions

We have observed the band gap narrowing of C-doped GaAs grown on GaAs substrates with various orientations. The temperature dependence of band-gap is well fitted by the Varshni equation. An empirical relation indicating the band-gap narrowing as a function of hole concentration is determined.

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References

- 1) D. Olego and M. Cardona, Phys. Rev. B **22** (1980) 886.
- 2) D. W. Shaw, J. Cryst. Growth **31** (1975) 130.
- 3) S. C. Jain, J. M. McGregor, and D. J. Roulston, J. Appl. Phys. **68** (1990) 2345.
- 4) B. E. Sernelius, Phys. Rev. B **34** (1986) 5610.
- 5) J.-S. Lee, I. Kim, B.-D. Choe, W. G. Jeong, Y. K. Sin, and W. S. Min, J. Appl. Phys. **79** (1996) 9278.
- 6) B. P. Yan, J. S. Luo, and Q. L. Zhang, J. Appl. Phys. **77** (1995) 4822.
- 7) S.-I. Kim, M.-S. Kim, S.-K. Min, and C. Lee, J. Appl. Phys. **74** (1993) 6128.