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Effect of Surface Morphology on the Density of Energy States in GaAsN grown by Chemical Beam Epitaxy

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1. Introduction

The $In_yGa_{1-y}As_{1-x}N_x$ semiconductor alloy is a promising material for ultra-high efficiency tandem solar cell, since its bang gap markedly decreases with increasing the N concentration in the film, without a significant change of lattice parameter. With only 3% of N and 9% of In, GaInAsN is a potential candidate for the lattice–matched tandem Ge (0.76 eV)/InGaAsN (1.04 eV)/GaAs (1.42 eV)/InGaP (1.89 eV) cell, which could achieve a conversion efficiency of more than 40% under standard AM0 radiation [1]. Meanwhile, incorporating a small atomic fraction of N in the alloy degrades markedly the lifetime and the mobility the both types of carriers [2], which consequently leads to decrease the diffusion lengths and limit the collection of photogenerated carriers in the solar cell device. An obvious reason of such degradation is the formation of active N-related recombination and scattering centers, owing to the large miscibility of the gap between GaAs and GaN, as well as to the smaller atomic size of N compared with its competitor atom for the same V-site. Experimentally, the distribution of the most energy states in the forbidden gap of GaAsN (The In source was not yet introduced in the growth of the alloy), grown by chemical beam epitaxy (CBE), was obtained by deep level transient spectroscopy (DLTS) [3]. Furthermore, some lattice defects were tentatively identified and their effects on the electrical properties of the material were partially clarified. The most important result related to defects in the alloy is the confirmation of the existence of an electron trap, with thermal activation energy between 0.3 and 0.4 eV below the conduction band minimum (CBM), which acts as a strong active N–related nonradiative recombination center [3]. It origin was tentatively suggested to be the split interstitial $(N\text{-}As)_{As}$. Furthermore, this recombination center was found to limit the lifetime of electrons during their transition to less than 0.3 ns. It is, therefore, essential to explore efficient ways to decrease the density of these defects by understanding their formation mechanisms and by optimizing the growth conditions. Recently, it was shown that the 311B GaAs substrate (B: with the component of [111] As orientation) enhances the N concentration and the photoluminescence (PL) properties in the alloy, as well as the lifetime of minority carriers, in contrast to Ga-terminal and conventional GaAs substrates [1]. Fundamentally, this result is related to the decrease of non-radiative recombination centers, however, this expectation has not yet been proved. For that, in this work, we carry out a comparison between the properties of lattice defects in GaAsN grown on GaAs 311B and conventional substrate by using deep level transient spectroscopy (DLTS) method and we correlate the results with the improvement of the optoelectronic properties of the alloy.

2. Experimental Procedure

Nominally two undoped GaAsN epilayers, labeled $GaAsN_{2AB}$, and $GaAsN_{311B}$, were grown by CBE system on high Zn-doped GaAs (001) 2AB, and GaAs (311) B (B-type: with the component of [111] As orientation), respectively at a growth temperature (T_G) of 440°C, a pressure of ~ 2 x 10^{-2} Pa, and a growth rate of 1.0 μm/h. Tridimethylaminoarsenic (TDMAAs = 0.5 sccm), Triethylgallium (TEGa = 0.05 sccm), and monomethylhydrazine (MMHy = 5.0 sccm) were used as Ga, As, and N chemical compound sources, respectively. The N concentrations were evaluated by high resolution X–ray diffraction (HRXRD) to be 0.354 % in $GaAsN_{2AB}$ and 0.376% in $GaAsN_{311B}$. The thicknesses of the epilayers were calculated to be 1253 nm and 1158 in $GaAsN_{2AB}$ and $GaAsN_{311B}$, respectively. Al and Au-Ge (88:12) dots with a diameter of 1 mm were evaporated ohmic contacts through a metal mask on the front of the samples, at a vacuum pressure of 10^{-4} Pa, and an alloy of Au-Zn (95:05) was deposited on the bottom surface as an ohmic contact. The type of conductivity and the density of carrier concentration were obtained by capacitance–voltage characteristics and from the fitting of the Mott–Schottky plots. The DLTS data were collected using a BIO–RAD digital DLTS system (DL8000). The activation energy E_T (eV) and the capture cross section σ_n (cm^2) of each recorded trap were determined from the slope and the intercept values of the Arrhenius plot of DLTS signal, respectively. For TR-PL measurement, a hetero-structure formed from a GaAs buffer layer with a thickness of 500 nm, a GaAsN layer with similar growth condition as the samples mentioned above, and a 30 nm GaAs cap layer. The lifetime of minority carriers was measured by using TR–PL method at room temperature. A mode–locked Ti: sapphire pulsed laser with a central wavelength of 800 nm was used as an excitation source. It generates pulses with a pulse width of less than 100 fs and a repetition rate of 80 MHz.

3. Results and Discussion

Illustrated in Fig. 1 are the DLTS spectra of electron traps in GaAsN grown on GaAs (001) 2° off toward [110] and GaAs (311) GaAs 311B. Six electron traps, E1 to E6,

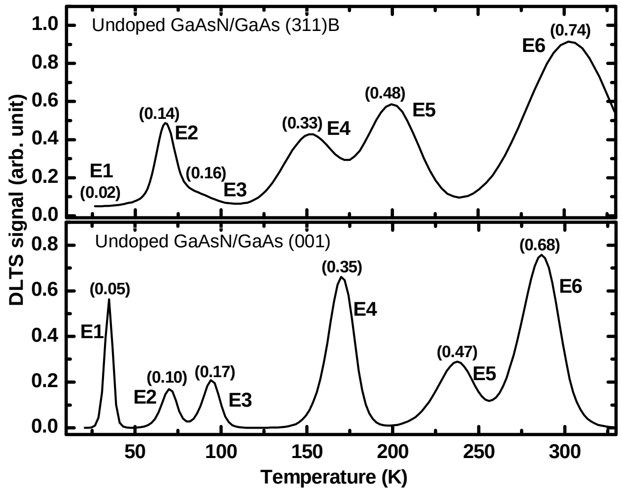

Fig. 1. DLTS spectra of GaAsN grown by CBE on GaAs (001) 2° off toward [110] (lower), and GaAs 311B (upper).

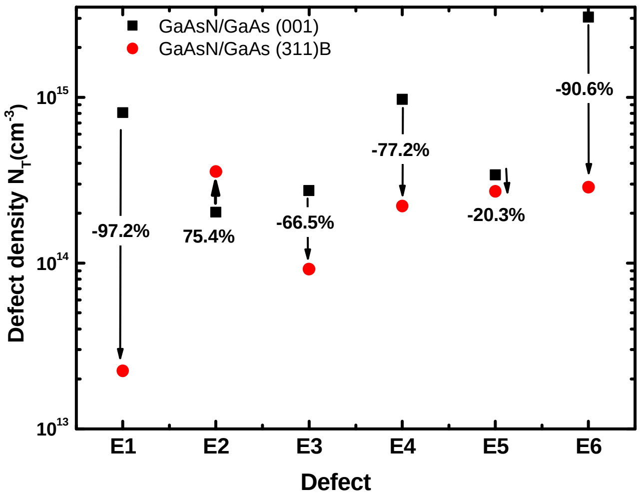

Fig. 2. Trapping densities of the electron traps E1 to E6 and their relative changes.

were recorded with apparent average activation energies of 0.04, 0.12, 0.16, 0.34, 0.45, and 0.73 eV below the bottom edge of the conduction band of GaAsN, respectively. Their trapping densities are plotted in Fig. 2 for the two kinds of substrates. Except E2, all the other electron traps showed a markedly decrease in their densities, ranging from 20.3 % for E5 to 97.2% for E1, despite the increase of the N concentration in $GaAsN_{311B}$. This interesting result is tentatively explained by the morphology of GaAs 311B, which is characterized by the abundance of three-dangling bond V-sites. Since the electronegativity of N is higher than that of As, the (311)B surface is therefore energetically preferable for N adatoms. Furthermore, it limits the As-related interstitial and substitutional defects. Another intersecting feature of this result is the decrease of the density of E4 up to ratio of 77.2 %. Since this electron trap was confirmed to act as N-related nonradiative recombination center, the dropping of its density is strongly suggested to be the main reason for the recovery of the optoelectronic properties of GaAsN grown on GaAs 311B. This improvement is clearly shown in Fig. 3, where the PL intensity and its decay in $GaAsN_{311B}$ are markedly higher than of that in $GaAsN_{2AB.}$ This indeed implies that the density of nonradiative recombination centers in GaAsN grown on GaAs 311B are quite lower than in GaAsN grown on conventional GaAs substrate.

4. Conclusions

The properties of electron traps in GaAsN alloys, grown on GaAs 311B and conventional 2AB substrates were studied and compared. Furthermore, the PL intensity and its decay were measured by TRPL method for the two samples. It was found that GaAs 311B is more suitable to decrease the density of nonradiative recombination centers in GaAsN grown by CBE, compared with GaAs 2AB substrate. This result was clearly observed in the enhancement of the PL intensity and the lifetime of minority carriers. Therefore, GaAs 311B is strongly expected to be more suitable to be used in solar cell application, as well as for recovering the electrical properties of GaAsN.

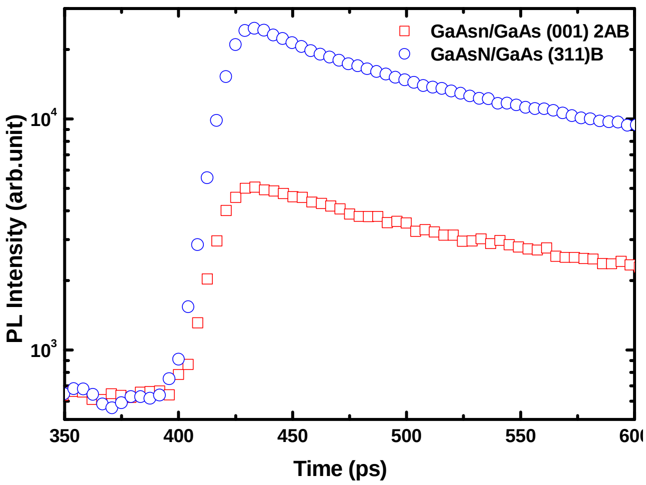

Fig. 3. PL decay of GaAsN grown on GaAs 311B and 2AB by CBE method.

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