Influence of potential fluctuation on optical and electrical properties in GaN

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We observed strong correlation between optical properties and transport properties in GaN. Both the intensity and the energy of near-band edge photoluminescence (PL) peak in GaN:Si vary with its mobility. Such behavior has been explained by the potential fluctuation associated with the inhomogeneous impurities or local defects, leading to the space-charge scattering of carriers and the redshift of the PL line. We also discuss the strain relaxation in GaN:Si. © *1998 American Institute of Physics.* [S0003-6951(98)00515-4]

Understanding optical and electrical properties of GaN is important for designing GaN-based optoelectronic and electronic devices. Both the optical parameters (e.g., absorption coefficient and radiation efficiency) and the electrical parameters (e.g., mobility) are associated with the scattering process of carriers. For example, impurities present in a crystal may reduce mobility as they act as scattering centers. They can also create electronic states within the band gap, allowing nonradiative recombination of electrons and holes. It is then of interest to study how the optical properties are related to the carrier transport in GaN.

Structural and optical properties of GaN:Si were studied by Ruvimov *et al.*[1] and by Lee *et al.*[2] Their study of photoluminescence (PL), Raman, and x-ray spectra suggests the reduced strain with increasing Si concentration [Si]. Schubert *et al.*[3] discussed the Si concentration dependence of the intensity and the width of the PL line at room temperature in GaN:Si. They attributed the increase of the linewidth with increasing [Si] to random potential fluctuation associated with ionized donors and acceptors. We discussed earlier that the fluctuating potential changes the well-defined impurity energy level into a broad impurity band[4] in GaN:Mg.[5] In this letter, we discuss how potential fluctuation influences both the electrical and optical properties in GaN:Si.

GaN:Si epilayers in this study were grown on sapphire substrates by metalorganic chemical vapor deposition (MOCVD), following low-temperature growth of GaN buffer layers. Si concentration was controlled by silane (SiH_4) flux. Photoluminescence was excited with the 325 nm line from a He–Cd laser. Unpolarized micro-Raman measurements were carried out at room temperature with an excitation wavelength of 5145 Å from an Ar^+ laser in a backscattering geometry.

Figure 1 shows the carrier concentration (n) and Hall mobility (μ) of the samples studied. Four samples (labeled 1a, 1b, 1c, and 1d) were grown under identical growth conditions except for silane flow. The GaN buffer growth rate for samples 2a–2d was reduced to half of that used for samples 1a–1d. For these samples the mobility increased with increasing n. Considering only the ionized impurity scattering, one expects the decrease of μ with increasing n, as shown by the dashed curve in the figure.

It was observed earlier that the mobility increased with increasing n up to $n \sim 10^{17}/\mathrm{cm}^3$, but decreased above it.[6–8] Ng *et al.*[6] attributed this to the combined effect of edge dislocation and ionized impurity scattering. In the model, the edge dislocations capture electrons and become negatively charged, thus scattering electrons. Hwang *et al.*,[7] on the other hand, attributed the anormalous behavior of mobility to the compensation by impurities such as carbon. In their study, the structural defect (except for nanopipes) was not found to be strongly related to mobility. Potential barriers at grain boundaries have been discussed by Hersee *et al.*[8] and Fehrer *et al.*[9] Whichever defect caused the mobility degradation in GaN, its influence on mobility will be more pronounced for smaller n, resulting in the decrease of μ with decreasing n.

A systematic increase of the PL intensity and the linewidth was observed with increasing n for samples 1a–1d and 2a–2d (not shown), similar to the result reported in Ref. 3. The full width at half maximum (FWHM) of the donor bound exciton line (I_2) at 15 K was 4.4 meV for sample 2a and 21.2 meV for sample 2d. The increase of 16.8 meV agrees well with the impurity broadening factor.[3]

For the rest of the samples, GaN buffer growth conditions (growth temperature, thickness, and growth rate of buffer layers) were varied, keeping the main growth condition and silane flow of 1.5 μmole/h. As seen in Fig. 1, the

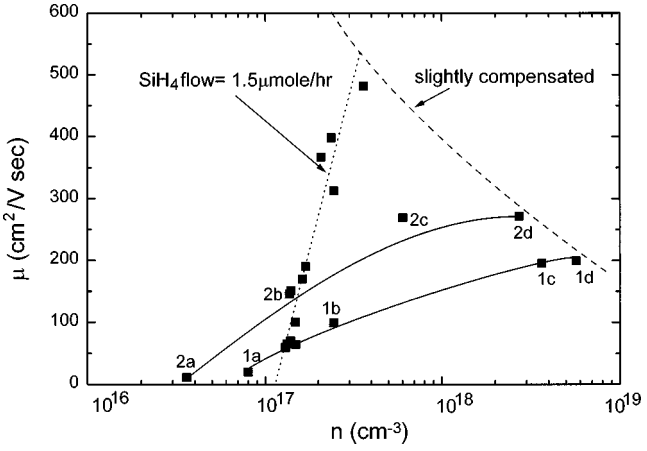

FIG. 1. Hall mobility (μ) and electron concentration (n) at room temperature. For constant Si concentration, mobility was found to vary with the buffer growth conditions.

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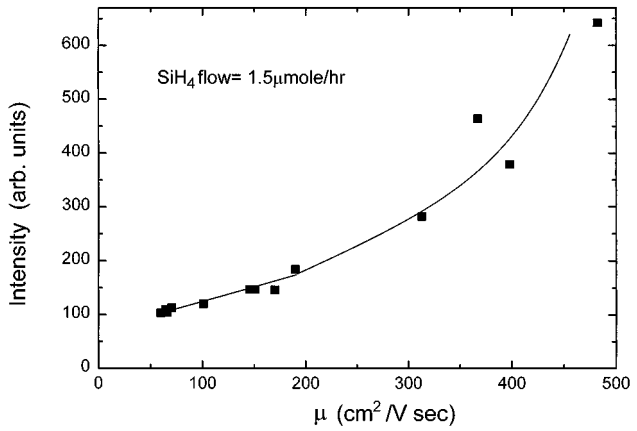

FIG. 2. The PL peak intensity at 300 K vs Hall mobility for GaN:Si for $n \sim 2\times10^{17}/\mathrm{cm}^3$.

carrier concentration increased from $1.4\times10^{17}/\mathrm{cm}^3$ to $3.6\times10^{17}/\mathrm{cm}^3$ with the increase of μ from 60 to 482 $\mathrm{cm}^2/\mathrm{V\,s}$, indicating the decrease of carrier compensation.

Figure 2 shows the increase of room-temperature PL intensity with the increase of Hall mobility for these samples. The increase of the intensity cannot be completely due to the increase of n since the increase of intensity is expected to be not more than 30% for the increase of n from $1.4\times10^{17}/\mathrm{cm}^3$ to $3.6\times10^{17}/\mathrm{cm}^3$, according to our plot of PL intensity vs n. It thus appears that the impurities and defects responsible for low Hall mobility also reduce the radiative recombination of photogenerated carriers.[10]

In general, various defects may influence electron transport and the following model is useful to consider possible factors affecting the mobility. In a perfect crystal, carriers will move without scattering in a periodic potential. The presence of point defects and structural defects alter the potential, resulting in the increase of carrier scattering or the decrease of mobility. The space-charge scattering due to inhomogeneous impurities and localized structural defects was taken into account to explain the empirical values of mobility.[11] For an ionized impurity concentration of $10^{18}/\mathrm{cm}^3$ and with a space-charge field of 20 kV/cm (corresponding to the band-edge fluctuation of 10 meV), mobility is expected to decrease from 500 to 200 $\mathrm{cm}^2/\mathrm{V\,s}$.

As implied in this model, not only the compensating acceptors such as carbon[12] and gallium vacancy[13] affect mobility in GaN:Si, but also any point defect or impurity may play an important role in determining carrier mobility. Antisite defects,[14] vacancies, and impurities such as oxygen[15] may produce lattice distortion, resulting in potential fluctuation. A potential barrier at grain boundaries[8,9] is an example of potential fluctuation by structural defects. Ionized donors and acceptors, other point defects, structural defects, and even lattice vibration (phonon) introduce band-edge fluctuation.

Figure 3(a) shows the peak energy of the donor-bound exciton line (I_2) at 15 K as a function of n. (Our undoped GaN layers are usually semi-insulating, but their typical I_2 energy is marked at $n=2\times10^{16}/\mathrm{cm}^3$ for convenience.) Shown in Fig. 3(b) are the relative Raman shifts of the E_2 phonon mode around $569\ \mathrm{cm}^{-1}$ with respect to the Raman frequency of the GaN:Si sample with $\mu=482\ \mathrm{cm}^2/\mathrm{V\,s}$. In Ref. 16, the E_2 phonon frequency is assumed to be a measure of strain since the mode does not strongly interact with electrons. The decrease of the PL energy and the Raman frequency with increasing [Si] was reported[1,2] and attributed to the strain relaxation.[17]

A plot of the I_2 energy versus Raman shift yields a slope of $5.7\ \mathrm{meV/cm}^{-1}$, which is much larger than that obtained from undoped GaN under biaxial strain.[18] In addition to the biaxial strain due to lattice mismatch and thermal strain observed in undoped GaN, GaN:Si may experience the decrease of lattice parameter due to the smaller atomic size of Si than that of Ga (or bond length of Si–N may be smaller than that of Ga–N). This will result in the hydrostatic strain relaxation and the decrease of band gap. However, the decrease of the I_2 energy is not only due to the ''shift of band edge'', but also due to the ''band-edge fluctuation'' associ-

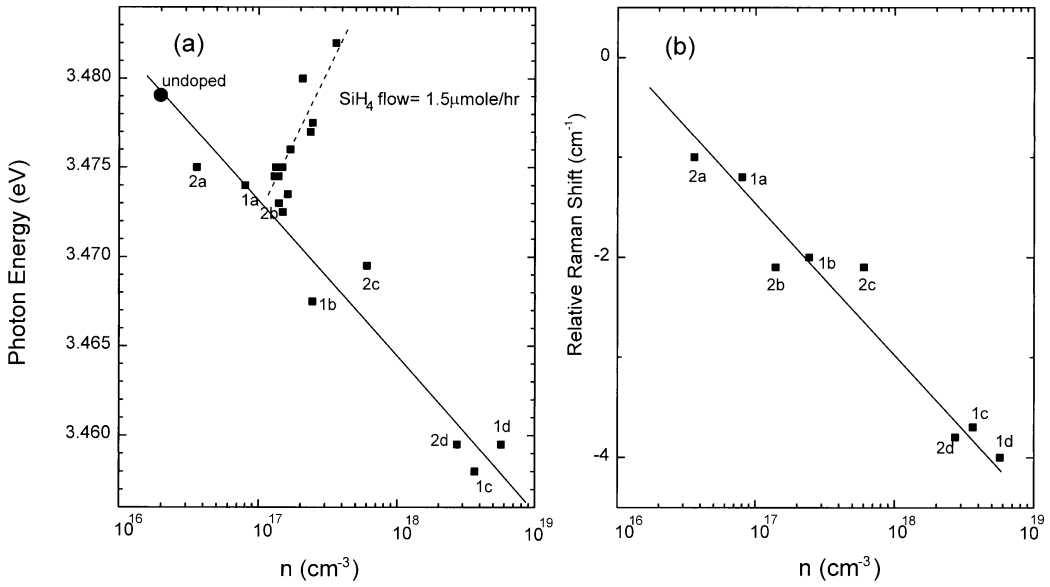

FIG. 3. The I_2 energy at 15 K (a) and relative shift of Raman frequency at 300 K (b) as a function of electron concentration. The dashed line shows that the I_2 energy varies even for constant [Si].

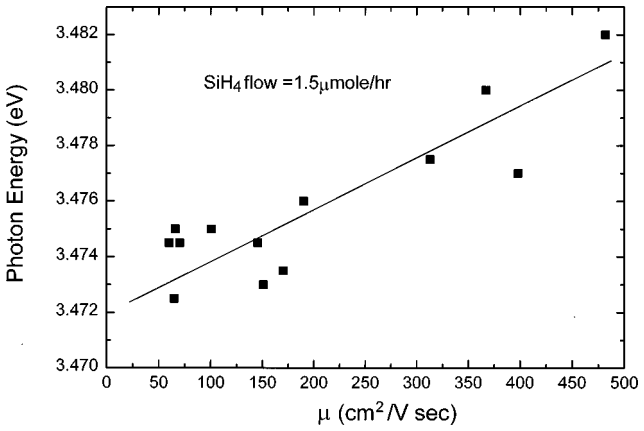

FIG. 4. The I_2 energy at 15 K as a function of Hall mobility for $n \sim 2 \times 10^{17}/\mathrm{cm}^3$.

ated with *local* strain. Similarly, the decrease of Raman shift with n may be partly attributed to the ''disorder-induced wave-vector nonconservation''.

If the increase of mobility is due to the decrease of potential fluctuation, the I_2 line is expected to blueshift with increasing μ even for constant [Si]. Such behavior is in fact manifested in Fig. 4, supporting the potential fluctuation model. Note that the I_2 energy of GaN:Si can be as high as 3.482 eV, even higher than the typical value for undoped GaN. It indicates that the biaxial strain of the sample is probably larger (or misfit dislocation density is smaller) than that of undoped GaN and that the strain relaxation due to Si incorporation is not significant up to $n \sim 2 \times 10^{17}/\mathrm{cm}^3$.

The local variation of impurities (including Si atoms) and defects may be responsible for the potential fluctuation in GaN:Si. With increasing [Si], the ''band-edge fluctuation'' will increase due to the increase of ionized donors, yielding the increase of linewidth and the redshift of the PL line. When the impurities and localized defects are reduced by growth optimization, potential fluctuation may decrease, leading to the increase of mobility and the blueshift PL line. This explains the larger slope of the I_2 energy versus Raman shift obtained from Fig. 3 and the redshift of the I_2 line with decreasing μ shown in Fig. 4.

We discussed the fact that the random distribution of impurities and defects may produce local strain and potential fluctuation. The large variation in PL energy with mobility as well as the impurity band formation[5] probably indicates that the potential fluctuation in GaN is larger than other semiconductors. Strong correlation between electrical properties and optical properties is observed in GaN and is explained by the potential fluctuation model.

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