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Photoreflectance investigation of band gap renormalization and the Burstein–Moss effect in Si doped GaN grown by MOVPE

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ABSTRACT

This work reports on the photoreflectance (PR) study of Si doped GaN layers (GaN:Si) with different doping levels (2.1×10^{17}–2.8×10^{19} cm^{-3}). GaN:Si samples have been successfully grown on sapphire substrate by metalorganic vapor phase epitaxy (MOVPE). Room temperature PR spectra showed Franz–Keldysh oscillation (FKO) features, reflecting the existence of a built-in electric field in the epilayers. The band gap energy determined using the FKO theory, is observed first to decrease and then to increase with increasing electron concentration. This result is explained by the competing effects of band gap renormalization and Burstein-–Moss band filling. Based on theoretical approach and experimental results, the interplay between these phenomena is systematically studied.

1. Introduction

GaN is the object of an increasing interest in the last few years owing to its potential applications in electronic and optoelectronic fields [1–4]. For the design and realization of GaN-based devices, high carrier concentration with a controlled and reproducible n- or p-type doping is needed [4]. Silicon (Si) is the primarily choice of the n-type dopant for GaN. It has been successfully used to produce films with free electron concentration higher than 10^{19} cm^{-3}. However, a considerable modification of the fundamental material parameters is often observed in heavily doped films [4,5]. Further improvements in high performance of GaN-based devices call hence for an accurate and systematic understanding of basic physical modification undergone by the material due to doping. In heavily doped semiconductor, one of the most important material parameter, namely the fundamental band gap, is frequently affected by high electron concentration as a result of a two competing effects [4–12]. First, the well-known Burstein–Moss (BM) band-filling effect, which shifts the absorption onset to higher energies with increasing carrier concentration [4–14]. The second phenomenon, called band gap renormalization (BGR), decreases the fundamental band gap energy with increasing carrier density due to many-body interactions [4–12,15]. Many papers were dedicated to the competing effects between BM band filling and BGR in III–V [12,16] and II–VI [8–11] semiconductors, using several theoretical models. Good agreement between theory and experiment has been achieved using a nonparabolic conduction band approximation [8–12]. For GaN, only little attention was paid to the interplay between BM and BGR effects. Furthermore, most of theoretical analyses about the optical band gap shift in GaN, assume the electron effective mass as a constant, based on parabolic band approximation [4,6,7,17]. However, the conduction band shows a nonparabolic nature in heavily doped material and the electron effective mass increases with carrier concentration [5,8–11,18]. For a complete understanding of the bandgap shift in doped GaN, an effective theoretical model which considers a nonparabolic conduction band is needed.

In this paper, PR spectroscopy, because of its high sensitivity, non destructive nature, and its precision in determining the optical transition compared to the conventional characterization methods [19–23], is used to study the interplay between BM band filling and BGR in Si doped GaN layers. A comprehensive comparison between experimental data and the available theoretical models is discussed. Using nonparabolic conduction band approximation, a good agreement between experimental results and theoretical calculation is obtained.

2. Experiments

Si-doped GaN epilayers were grown by MOVPE on (0001) sapphire substrates in a vertical reactor at atmospheric pressure. Trimethylgallium (TMG), ammonia (NH_3) and silane (SiH_4) diluted

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Table 1
Summary of epilayer thickness, electron concentration (n), lattice parameters (a and c), energy gap values obtained from PR (E_g), energy shifts due to strain (ΔE_s), and resulting corrected energy gap values (E_{gcor}) using Eq. (2).

	Thickness (μm)	n (cm^{-3})	a (Å)	c (Å)	ΔE_s (meV)	E_g (eV)	E_{gcor} (eV)
S1	2	2.1×10^{17}	3.1862	5.1867	+10	3.419	3.409
S2	2.6	6.9×10^{17}	3.1880	5.1857	+4	3.409	3.405
S3	2.2	2.1×10^{18}	3.1908	5.1843	−6	3.398	3.404
S4	1.7	6×10^{18}	3.1917	5.1841	−8	3.400	3.408
S5	1.1	1.8×10^{19}	3.1912	5.1842	−7	3.418	3.425
S6	1.1	2.8×10^{19}	3.1911	5.1842	−7	3.438	3.445

in 500 ppm of H_2 were used as the precursors of gallium, nitrogen, and silicon, respectively. After a substrate surface cleaning procedure, typical experiment begins by heating the sapphire substrate under a mixture flow of H_2+NH_3 at 1050 °C for 10 min. Then the temperature was lowered to 600 °C in order to deposit the GaN buffer/nucleation layer. After a temperature ramp from 600 to 1080 °C, the GaN:Si epilayer were finally grown by the simultaneous introduction of TMG and SiH_4 into the reactor. SiH_4 flow rate has been varied in order to obtain different Si doping level. The growth rate and film thickness were monitored in-situ by diode laser reflectometry at 633 nm [24]. Hall measurements and high-resolution X-ray diffraction were used to determine the carrier concentration (n) and the lattice parameters (a and c) of the obtained samples, respectively. All results are reported in Table 1. PR measurements were carried out by employing a standard setup with the 325 nm line of He–Cd laser as the pump light which was mechanically chopped at 280 Hz. The probe light was obtained from a 75 W Xe lamp dispersed with a 275 mm focal length monochromator. The reflected light was detected by an UV-enhanced Si photodiode operating in photovoltaic mode.

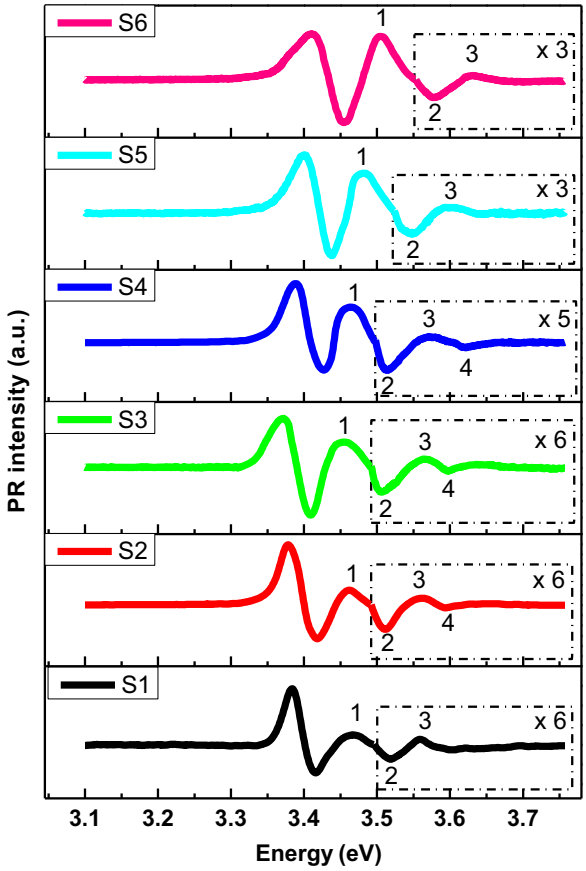

Fig. 1. Room temperature photoreflectance spectra of Si doped GaN layers with different Si doping level. The appearance of FKO above the GaN bandgap energy indicates the existence of a strong electric field in the layers.

3. Results and discussion

3.1. Experimentally measured band gap

Fig. 1 shows room temperature photoreflectance spectra measured for Si-doped GaN layers. All spectra show fringes above the GaN bandgap energy, which are attributed to the Franz–Keldysh effect [21–23]. The FKO features are related to the modulation of the built-in electric field in surface layer or/and in the space charge region due to junction between epitaxial layer and substrate [22,23]. To evaluate the band gap energy of the films, the FKO period is analyzed within the asymptotic expression for PR [21,22]. According to this model, the energy of oscillation extrema (E_m) is given by:

$$E_m = (\hbar\theta)H_m + E_g \quad (1)$$

with $H_m = \left[\left(\frac{3\pi}{4}\right)\left(m-\frac{1}{2}\right)\right]^{\frac{2}{3}}$, $\hbar\theta$ is the electro-optic energy, E_g the band gap energy and m denotes the mth FKO extremum. According to Eq. (1), the plot of E_m against H_m shows a linear relationship and its intercept yields the band gap E_g. The FKO analyses are shown in Fig. 2, where the straight lines represent the least-squares fit to Eq. (1). The obtained band gap energies are summarized in Table 1. We observe a clear dependence of the band gap energy on the Si doping level. Indeed, the band gap energy decreases from 3.419 to 3.398 eV as the electron concentration increases from 2.1×10^{17} to 2.1×10^{18} cm^{-3}. Above 2.1×10^{18} cm^{-3}, the band gap energy increases with n to reach the value 3.438 eV for an electron concentration of about 2.9×10^{19} cm^{-3}. The variation of the band gap energy with Si doping level is ascribed to the competing effects between BGR and BM, and to the strain induced band gap shift caused by the Si dopant atoms. To accurately evaluate the interplay between BGR and BM, it is necessary hence to correct the value of the measured energy band gap by removing the contribution of strain. In connection with the current study, the strain-dependent energy corrections ΔE_s are calculated as follows [4,25–27]:

$$\Delta E_s = E_g - E_{gcor} = (a_1 - D_3)\varepsilon_{zz} + 2(a_2 - D_4)\varepsilon_{xx} \quad (2)$$

where, E_g is the band gap energy of strained material, and E_{gcor} is the resulting corrected energy. a_1, a_2, D_3 and D_4 are the interband hydrostatic deformation potentials and the valence band deformation potentials constants, respectively. $\varepsilon_{xx} = \frac{a-a_0}{a_0}$ is the in-plane strain, while $\varepsilon_{zz} = \frac{c-c_0}{c_0}$ is the strain along the c-axis. $a_0 = 3.1892$ Å and $c_0 = 5.1852$ Å are the unstrained bulk GaN lattice parameters [28]. Here we take the values of a_1, a_2, D_3 and D_4 to be −3 eV, −12.4 eV, −9.4 eV and −4.7 eV, which are accurately determined by Fu et al. using more precise results obtained from high-quality strain-free GaN films [26]. It should be emphasized that these values are somewhat different from the ones determined recently by Ishii et al. [29] using reflectance measurements. However, we believe that this difference does not have a crucial impact on the accuracy of our model. Using the mentioned deformation potentials values, ΔE_s and E_{gcor} are calculated and the results are summarized in Table 1. The sign change in the energy correction ΔE_ss reveals a transition of the residual stress state in Si-doped GaN films from compressive to tensile as observed in earlier studies [17,30].

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