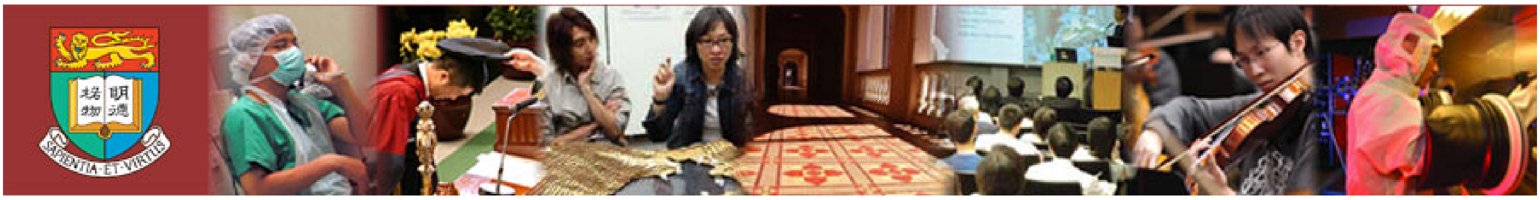

Title	**Stress and its effect on optical properties of GaN epilayers grown on Si(111), 6H-SiC(0001), and c-plane sapphire**
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Stress and its effect on optical properties of GaN epilayers grown on Si(111), 6H-SiC(0001), and *c*-plane sapphire

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The stress states in unintentionally doped GaN epilayers grown on Si(111), 6H-SiC(0001), and *c*-plane sapphire, and their effects on optical properties of GaN films were investigated by means of room-temperature confocal micro-Raman scattering and photoluminescence techniques. Relatively large tensile stress exists in GaN epilayers grown on Si and 6H-SiC while a small compressive stress appears in the film grown on sapphire. The latter indicates effective strain relaxation in the GaN buffer layer inserted in the GaN/sapphire sample, while the 50-nm-thick AlN buffer adopted in the GaN/Si sample remains highly strained. The analysis shows that the thermal mismatch between the epilayers and the substrates plays a major role in determining the residual strain in the films. Finally, a linear coefficient of 21.1 ± 3.2 meV/GPa characterizing the relationship between the luminescent bandgap and the biaxial stress of the GaN films is obtained. [DOI: 10.1063/1.1592306]

GaN and related nitrides represent a class of wide band gap semiconductors, which have attracted much attention due to their promises in blue and ultraviolet light emitting device applications.[1] Since sizable nitride substrate is not yet available GaN is commonly grown on foreign substrates, among which, sapphire and SiC are two major ones. Very recently, Si is gaining more interest as an alternative substrate because of its low-cost, large wafer size, and high crystal quality. In fact, crack-free GaN epifilms have already been demonstrated on Si.[2–5] The knowledge of strain or stress state in epitaxial GaN is very important for better understanding film's property and improving nitride-based devices. As a sensitive, local and nondestructive tool, Raman scattering spectroscopy has been widely employed to measure stress or strain in semiconductor heterostructures.[6] In the past a few years, Raman scattering measurements for residual strain in GaN epilayers grown on sapphire have been reported.[7–12] There are few studies devoted to investigating stress state in GaN films grown on SiC and Si.[13–15]

In this letter, the residual stress in GaN grown on Si(111), SiC(0001), and *c*-plane sapphire was investigated and compared using confocal micro-Raman scattering technique. It is found that a strong tensile stress exists in GaN film grown on Si, while for film grown on sapphire, a small compressive stress is detected. Adopting the stress coefficients reported in literature, the amounts of residual stress in the samples are calculated from the measured frequency shifts of the E_2-high mode in Raman spectra. Photoluminescence (PL) spectra from the samples are also measured at room temperature. A linear relationship between the stress and luminescent band gap is observed.

The GaN/Si and GaN/sapphire samples were grown by metalorganic chemical vapor deposition, while the GaN/6H-SiC samples were prepared by molecular-beam epitaxy. In growing GaN on Si(111) substrate, a ~50-nm-thick AlN buffer layer was firstly deposited prior to growing the top GaN layer at 1100 °C. For samples on sapphire, a ~30-nm-thick GaN buffer was inserted between the substrate and the top GaN layer. For GaN/SiC(0001), there is no buffer layer and the epifilm was directly grown on substrate at 650 °C. The thicknesses of the epifilms are in a range of 2–5 μm. All samples are unintentionally doped. Raman scattering experiments were carried out in a backscattering geometry with a combination of instruments of monochromator equipped with 1800 lines/mm grating, microscope, charge coupled device detector cooled by liquid nitrogen, and a notch filter. In the room-temperature Raman scattering experiments, the 488 nm line of Coherent $Ar^+ + Kr^+$ mixed gas laser was employed as the excitation light and a 100× objective lens was used in the confocal microscope to focus and collect the laser light before and after scattering. Under these conditions, the spatial resolution of the instrument is about 1 μm. The PL setup used in the present work has been described elsewhere.[16] Standard lock-in amplification was employed in the PL measurements.

Figure 1 shows the Raman spectra of the three samples at room temperature. Consistent with literature reports, both the E_2-high and A_1-LO modes are observed. It is also seen that their positions are substrate dependent, implying different stress states in different samples. Besides these two main peaks, several other weak peaks are present in the spectrum from GaN/Si sample. In the semilogarithmic plot of Fig. 2, Raman spectra from GaN/Si and from a Si reference sample are compared. It shows that the peaks at 619 and 669 cm^{-1} are from the Si substrate as confirmed also by Tripathy *et al.*[14] On the other hand, the peak at 649 cm^{-1} cannot be associated with the Si substrate. We assign this peak to be the

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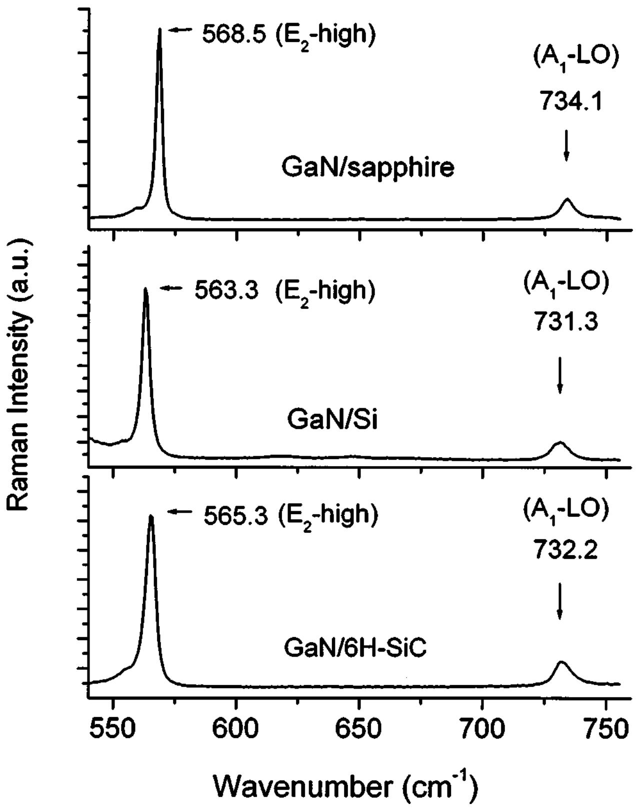

FIG. 1. The room-temperature Raman spectra measured from the GaN/Si(111), GaN/sapphire, and GaN/6H-SiC samples.

E_2-high mode of the AlN, which is the buffer layer in the sample. The peak position, however, deviates from the characteristic frequency of 655 cm^{-1} for an unstrained AlN,[17–19] which means that the AlN layer subjects to a tensile strain in the sample.

In the linear approximation, the deviation in frequency of a given phonon mode γ under symmetry-conserving stress can be expressed in terms of the biaxial stress σ_{xx}:[20,21]

$$\Delta\omega_{\gamma} = \mathrm{K}_{\gamma}\sigma_{xx}, \tag{1}$$

Obviously, the biaxial stress can be calculated, according to Eq. (1), from the measured Raman frequency shift of a given phonon mode if the linear stress coefficient K_γ is known. Very recently, Gleize *et al.*[21] have reported a stress coefficient of 3.39 cm^{-1}/GPa for the E_2-high mode of AlN, which falls in between the values reported respectively by Prokofyeva *et al.* (4.5 cm^{-1}/GPa)[22] and by Sarua *et al.* (3.0 cm^{-1}/GPa).[23] We adopt here the Gleize *et al.*'s value for the stress coefficient and a standard frequency of 655 cm^{-1} for AlN E_2-high mode. The calculated residual stress in the AlN buffer layer is approximately 1.77 GPa.

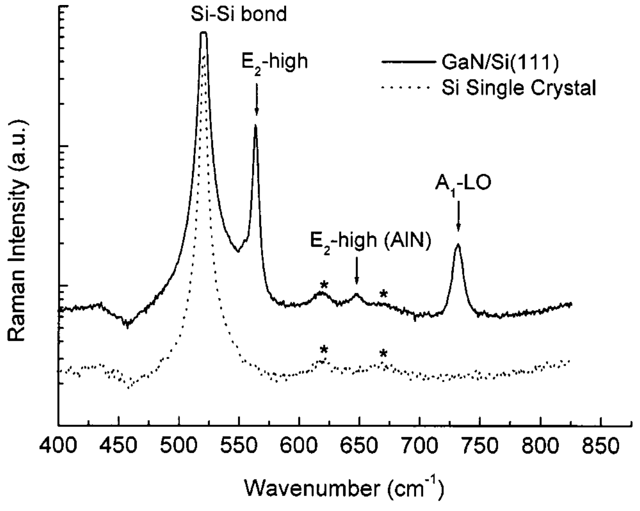

FIG. 2. The semilogarithmic Raman spectra from the GaN/Si (solid line) and from the Si reference sample (dotted line). Asterisks mark the signals from the Si substrate.

We now examine the stress states in GaN layers grown on various substrates. The E_2-high modes in the Raman spectra (Fig. 1) are used for this purpose because it has been proven particularly sensitive to biaxial stress in GaN epifilms.[24] For the GaN/Si sample, the stress coefficient 4.3 cm^{-1}/GPa reported by Tripathy *et al.*[14] is adopted and the calculated stress in the top GaN layer is 1.09 GPa. The stress is tensile because its E_2-high peak exhibits a red shift of 4.7 cm^{-1} with respect to the standard value of 568 cm^{-1} for bulk GaN.[24] Concerning the GaN epilayer directly grown on 6H-SiC, the residual stress is estimated to be 1.0 GPa, where the stress coefficient is taken to be 2.7 cm^{-1}/GPa according to Refs. 13 and 20. Similar to GaN epifilm on Si, the stress in GaN grown on SiC is also tensile.[13,24] For GaN epilayers grown on sapphire, the value of stress coefficient for the E_2-high mode are considerably scattered in the literature.[24] Here, we adopt a theoretical value of 2.56 cm^{-1}/GPa as given by Wagner and Bechstedt[20] to calculate the residual stress. A small compressive stress of ~0.2 GPa is found for the sample, whose Raman spectrum is shown in Fig. 1 (top curve). Referring to the material parameters,[25] it is not difficult to understand why an opposite stress states exist in GaN epilayers grown on Si versus on sapphire. For GaN/Si system, the lattice constant of GaN is smaller than that of Si [the atomic spacing on the (111) plane of Si is 3.84 Å] and its thermal expansion coefficient is larger than that of Si. Both lattice and thermal mismatches lead to the tensile stress in the GaN epilayer. For the case of GaN/sapphire, it is known that the lattice of epitaxial GaN rotates by 30° with respect to that of sapphire, and so the atomic spacing of the substrate parallel to **a** of GaN is only 2.75 Å (see Ref. 26). Consequently, epitaxial GaN layer is expectedly compressively stressed. For sample GaN on SiC, both lattice and thermal mismatches between the epilayer and the substrate are relatively small, where the lattice constant of GaN is slightly larger than that of SiC. It is thus somewhat surprising to observe the relative larger stress present in GaN and evermore, the stress is tensile. We attribute such a result to the effect of thermal expansion.[25] Stress is built in film during sample cooling from deposition temperature to room temperature after growth and this stress can overcompensate that due to lattice constant mismatch in this case. Our transmission electron microscopy and *in situ* reflection high energy electron diffraction observations show that the misfit stress due to lattice constant difference between GaN and 6H-SiC is partly relieved through generation of dislocations.

It is known that the energy bandgap of a semiconductor is affected by the residual stress in film. A tensile stress will result in a decrease of energy band gap while a compressive strain causes an increase of the band gap. Figure 3 shows a set of PL spectra for the same three samples as used for Fig. 1. They are measured at room temperature. Figure 4 depicts

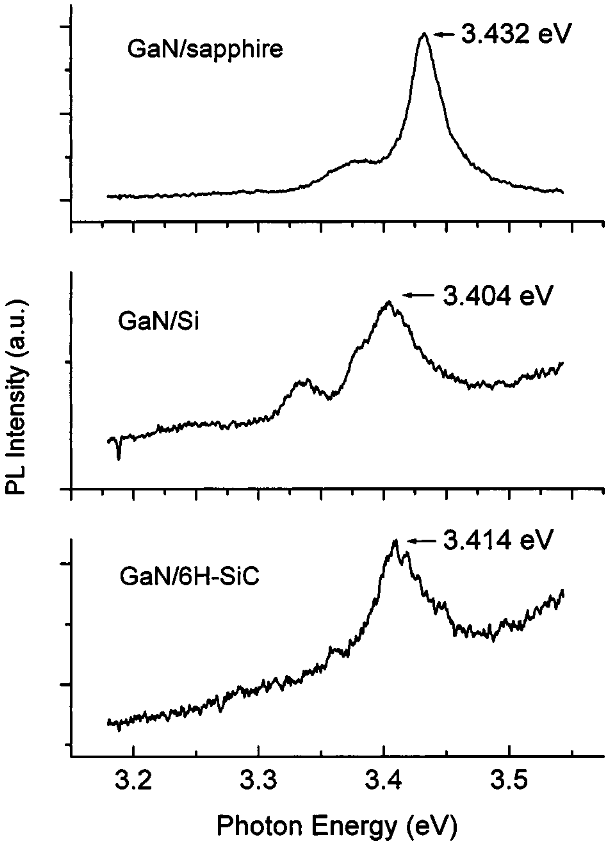

FIG. 3. The room-temperature photoluminescence spectra of the GaN/sapphire, GaN/Si(111), and GaN/6H-SiC.

the luminescent band gap as represented by the PL peak positions versus residual stress in film for five samples, two are GaN/SiC, another two are GaN grown on sapphire and the other one is on Si. An approximate linear dependence is observed. By least-square fitting of the data, the bandgap of GaN at room temperature can be expressed in terms of biaxial stress according to

$$E_g = 3.4285 + 0.0211\sigma_{xx}(\mathrm{eV}). \tag{2}$$

In summary, we have investigated room-temperature Raman and PL spectra of GaN epilayers grown on sapphire, Si(111) and 6H-SiC(0001) substrates and derived the stress states in films. It is found that the thin GaN buffer layer grown at low temperature effectively relieves the strain in GaN/sapphire, while AlN buffer layer inserted between Si(111) and the top GaN epifilm remains highly strained. The thermal stress can also play a key role in deciding the residual strain in film, as demonstrated for the case of GaN grown on SiC. A linear relationship of the luminescent band gap of GaN with the residual stress in film at room temperature is observed, and a linear coefficient of 21.1 ±3.2 MeV/GPa is derived.

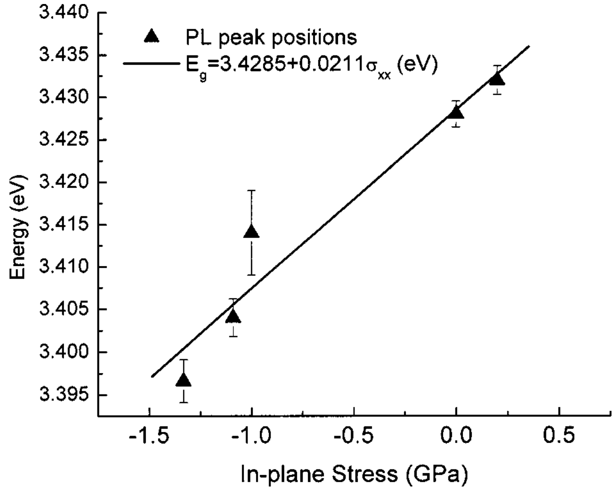

FIG. 4. The room-temperature luminescent band gaps of the GaN epilayers vs the corresponding stresses. The solid line represents a linear fitting result to the experimental data.

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