IR reflection of optical phonons in GaN/AlGaN superlattices


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We present the IR study of vibrational properties of GaN/Al0.28Ga0.72N superlattices with different thickness of superlattice layers. IR reflection spectra of the superlattices were taken at normal and off-normal incidence using p-polarised light in order to analyze optical phonons propagating both along and perpendicular to the layer surface. Optical phonon frequencies as well as thickness of the structure layers were determined from a comparison of the experimental IR reflection spectra to those calculated in the framework of the dielectric continuum model.

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1 Introduction The group-III nitrides such as GaN, AlN and AlxGa1-xN solid solutions attract much attention for application in high-power, high-frequency and high-temperature electronics and optoelectronic devices. GaN/AlGaN multiple quantum wells and superlattices (SLs) are considered as perspective materials for the devices with optimized performance. In addition, to their device application GaN/AlGaN SLs possess unique physical properties which are of particular interest for basic investigations. Among them, vibrational properties of the wurtzite superlattices which are different from those of the SL constituents, play a crucial role in electron-phonon interaction which may lead to device degradation. However, up to now, the knowledge of the most fundamental properties of GaN/AlxGa1-xN SLs is still relatively poor and, in particular, little is known about their vibrational properties.

Raman spectroscopy is a commonly used technique for investigation of vibrational properties of the group-III nitrides (Ref. [1] and references therein). Recently, a number of research groups has published the results of their Raman studies of GaN/AlGaN quantum wells and superlattices [2–8]. Infrared reflectance (IR) is an efficient, complementary to Raman spectroscopy and non-destructive method to determine the optical and structural details of a layered system [9]. Recently, IR spectroscopy was also applied to study GaN and AlxGa1-xN epilayers [10, 11]. As far as we know the only paper devoted to IR study of GaN/AlN superlattices was published [12]. The present paper reports the IR study of optical phonons in GaN/AlGaN superlattices which have not been investigated yet.

2 Experimental The GaN/Al0.28Ga0.72N superlattices studied were grown by MOCVD on (0001)-oriented sapphire substrates using a redesigned Epiguiq VP-50 RP system with a horizontal flow quartz reactor and an inductively heated graphite susceptor [13]. The samples consisting of 74, 148, 296 and 370 periods (samples A, B, C and D, respectively) of GaN and Al0.28Ga0.72N with nominal thicknesses of 20 nm, 10 nm, 5 nm, 2.5 nm were fabricated on a GaN buffer layer at the substrate temperature of 420 °C.

The IR reflection spectra were recorded using FTIR spectrometers Bruker IFS-113v in the spectral range of the optical lattice vibrations of the GaN and AlN (400–1400 cm⁻¹) at a temperature of T = 80 K.

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Spectra were taken at normal incidence of IR light and at off-normal incidence (θ ≈ 70°) using p-polarized light in order to analyze both the transverse optical (TO) and longitudinal optical (LO) vibrational modes in thin layers [14]. The resolution was 1 cm⁻¹ over the whole spectral range. The number of scans was 1000. IR reflection spectra of a bare sapphire substrate were measured in the same conditions and further used to determine the optical parameters of the sapphire.

3 Results and discussion

Figure 1 show experimental IR spectra of the samples A and B measured at normal (Fig. 1a and Fig. 1c) and off-normal incidence using p-polarized light (Fig. 1b and Fig. 1d), respectively. Several features can be seen in Fig. 1 which are either interference fringes or overlapping of several modes from sapphire substrate, GaN buffer and the rest phonon modes in the SLs. In order to understand the experimental spectra IR reflection spectra of an anisotropic sapphire substrate and the superlattices (samples A-D) were calculated.

In the long-wavelength approximation (when λ ≫ d₁ and λ ≫ d₂, where λ is the wavelength of the IR light, d₁ and d₂ are the thicknesses of the SL layers) the dielectric response function of the samples under investigation can be presented as a tensor

\[ \varepsilon(\omega) = \begin{pmatrix} \varepsilon_{z}(\omega) & 0 & 0 \\ 0 & \varepsilon_x(\omega) & 0 \\ 0 & 0 & \varepsilon_y(\omega) \end{pmatrix} \]

where the z axis is normal to the layers and \( \varepsilon_z(\omega) = \varepsilon_{\perp}(\omega) \). The components of dielectric function (1) are commonly described by the model of damped harmonic oscillator for each IR active phonon branch:

\[ \varepsilon_{x,y}(\omega) = \varepsilon_{x,y}(\omega) + \sum_i \frac{A_{x,y} \cdot \omega_{x,y,TO} \cdot \omega_{x,y,L}}{\omega_{x,y,TO}^2 - \omega^2 - i \gamma_{x,y,i}} \]

Here \( \varepsilon_{\perp}(\omega) \) denotes the surface normal direction whereas \( \varepsilon_{x,y}(\omega) \) indicates the optical constants in the
plane of the interfaces, \( \varepsilon_{\infty}, A_1, \omega_{TO}, \) and \( \gamma \) are the corresponding high-frequency dielectric constants, the amplitudes, the resonance frequency of the \( i \)th TO-phonons propagating in \( x \) or \( z \) directions and their broadening, respectively. IR reflection spectra of anisotropic structures were calculated using WVASE 32 program [15]. Details of calculations of IR reflection spectra of anisotropic samples can be found in Ref. [16, 17].

In order to calculate the optical parameters of the superlattices the IR spectra of a bared sapphire substrate were calculated. This task itself is considered as a sophisticated problem and was solved only recently [16]. The results of our calculation presented in Table 1 are in accordance with those presented in Ref. [17]. From comparison of the IR spectra of a sapphire substrate with those of samples A-C one can conclude that the shape of the IR spectra of the GaN/AlGaN SLs is strongly influences by reflection from the sapphire substrate. Qualitatively, the features below 500 cm\(^{-1}\) are determined by phonon lines from sapphire substrate influenced by interference on the total sample and/or SL thickness. All other features observed in Fig.1 are most probable interference fringes or overlapping of several modes from sapphire substrate, GaN buffer and the rest phonon modes in the SLs. Therefore, a direct determination of phonon frequencies from IR reflection spectra leads to erroneous results and, thus, an adequate model calculation of layered structure is strongly needed.

Using the calculated parameters for sapphire, the IR spectra of the GaN/AlGaN SLs were simultaneously fit to the experimental spectra measured in normal and off-normal incidence. Each layer was

\[
\begin{array}{|c|c|c|c|c|}
\hline
\text{material parameter} & \text{Sapphire} & \text{GaN buffer} & \text{GaN SL layer} & \text{Al}_{0.23}\text{Ga}_{0.72}\text{N SL layer} \\
\hline
D, \text{ nm} & 410 & A & 750 & 20 \\
 & & B & 950 & 10.8 \\
 & & C & 800 & 6 \\
 & & D & 550 & 2.5 \\
\hline
\varepsilon_{\infty} & 3.077 & 5.35 & 5.35 & 5.19 \\
\hline
\omega_{TO}, \text{ cm}^{-1} & 385 & 558 (E_1(\text{TO})) & 567 (E_1(\text{TO})) & 635 (E_1(\text{TO}) \text{ AlN-like}) \\
\hline
A_1, \text{ cm}^{-1} & 8.4 & 2300 & 2750 & 650 \\
\gamma_1, \text{ cm}^{-1} & 7 & 6 & 1.8 & 55 \\
\hline
\omega_{TO}, \text{ cm}^{-1} & 439.1 & 570 (E_1(\text{TO}) \text{ GaN-like}) & 570 (E_1(\text{TO}) \text{ GaN-like}) & 1600 \\
\hline
A_2, \text{ cm}^{-1} & 1262.7 & 127.98 & 4 \\
\gamma_2, \text{ cm}^{-1} & 3.05 & 5.56 & 1.58 \\
\hline
\omega_{TO}, \text{ cm}^{-1} & 569 & 633.6 & 3.49 & 582.4 \\
\hline
A_3, \text{ cm}^{-1} & 1728 & 127.98 & 8 & 7.17 \\
\gamma_3, \text{ cm}^{-1} & 5.56 & 7.17 & 5.35 & 5.35 \\
\hline
\varepsilon_{\infty} & 3.072 & 5.35 & 5.35 & 5.19 \\
\hline
\omega_{TO}, \text{ cm}^{-1} & 398 & 533 (A_4(\text{TO})) & 538 (A_4(\text{TO})) & 544 (A_4(\text{TO}) \text{ GaN-like}) \\
\hline
A_4, \text{ cm}^{-1} & 2678 & 2650 & 2600 & 3300 \\
\gamma_4, \text{ cm}^{-1} & 3.49 & 8 & 5 & 10 \\
\hline
\omega_{TO}, \text{ cm}^{-1} & 582.4 & 976.26 & 1.58 & \\
\hline
\end{array}
\]

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treated as anisotropic one. Comparison of the experimental and calculated spectra is shown in Fig. 1. One can see a very good agreement of experimental data with the results of calculations. The calculated optical phonon and structural parameters of SL layers and GaN buffer are presented in Table 1. The assignment of transverse optical phonons in the SL layers according to their symmetry is also given in Table 1. The frequency positions of both $E_1$(TO) and $A_1$(TO) phonons in GaN buffer (558 and 533 cm$^{-1}$, respectively) determined from the fitting procedure are in accordance with the Raman data [18]. The $E_1$(TO) and $A_1$(TO) phonon frequency positions in GaN SL layers are shifted toward the higher frequencies due to compressive strain in the layers [19]. The frequency positions in AlGaN SL layers are modified by two-mode behavior of TO phonons and tensile strain in the layers. Therefore, the $E_1$(TO) AlN-like at 635 cm$^{-1}$ and $E_1$(TO) and $A_1$(TO) GaN-like phonons (at 570 and 544 cm$^{-1}$, respectively) are active in the IR spectra. It is worth mentioning that IR spectra of all samples were best fit using the same optical phonon parameters. Beside the optical phonon parameters the structural parameters of the samples such as the thickness of GaN buffer layer and SL layers were determined. One can see that the overall SL period for samples B and C exceeds the nominal SL period. The validity of the parameters obtained in proven by diffraction data [19].

In conclusion, IR spectra of GaN/Al$_{0.28}$Ga$_{0.72}$N superlattices measured in both normal and off-normal incidence were described with dielectric function model of anisotropic layered structure. Optical phonon and structural parameters determined from comparison of the calculated and experimental IR spectra are in good agreement with data of Raman and diffraction experiments.

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References