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Plasmon phonon modes and optical resonances in $n$-GaN

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Abstract. We study theoretically and experimentally transverse and longitudinal electromagnetic waves in $n$-GaN epitaxial layers. The studies are carried out on the epitaxial layers with various doping levels. Simulation of the reflectivity and absorptivity spectra is performed in a wide frequency range. Additionally, the radiation emission spectra are simulated for various temperatures of the GaN epitaxial layer. It is shown that the resonance peculiarities of the optical spectra are located closely to the frequencies of the coupled plasmon phonon modes. Experimental studies of the reflectivity spectra have been performed in the spectral range 2–20 THz. The experimental spectra are well fitted by the simulated ones and can be used for contactless determination of the electron concentration and mobility in GaN epitaxial layers. The experimental and theoretical results of the present work provide insights for the development of GaN-based devices aimed to absorb/emit terahertz or mid infrared radiation selectively.

1. Introduction

Gallium nitride is one of the most promising materials for applications in terahertz (THz) and mid infrared photonics. Various micro- and nanostructures based on GaN are used as THz detectors and emitters. The number of different physical effects used in these devices is constantly growing. In particular, one can mention the following recent investigations related to THz radiation emission in gallium nitride: THz radiation emission due to intracenter optical transitions in lightly doped $n$-GaN epitaxial layers [1], thermal radiation of hot electrons in the THz range in a single heterojunction AlGaN/GaN [2], THz emission due to plasmon excitation in GaN/AlGaN HEMT structures with submicron gate length [3], THz emission associated with surface plasmon polaritons in GaN-based microstructures [4]. It is feasible to obtain selective THz radiation emission/detection by means of bulk plasmon phonon polaritons in $n$-GaN epitaxial layers. To this end, in the present paper we investigate the optical properties of $n$-GaN/sapphire microstructures. In addition to transverse electromagnetic waves, longitudinal electromagnetic waves in $n$-GaN are also examined.

The plasmon–LO phonon interaction, i.e. an interaction between a longitudinal electromagnetic wave caused by free electron displacement relative to the positive background and longitudinal optical (LO) lattice vibrations, becomes significant when the plasma frequency $\omega_p = \left(\frac{4\pi^2N_e}{\varepsilon m_e}\right)^{1/2}$ is
comparable with the LO phonon frequency $\omega_{LO}$ where $e$ and $m_e$ are the electron charge and the effective mass, respectively, $N_e$ is the free electron concentration, $\varepsilon_\infty$ is the high frequency permittivity. Firstly, we calculate the concentration dependence of the frequencies of the coupled plasmon–LO phonon modes which represent longitudinal electromagnetic waves. Secondly, we consider a few certain values of electron concentration corresponding to three frequency ranges, namely $\omega_p < \omega_{LO}$, $\omega_p \approx \omega_{LO}$, and $\omega_p > \omega_{LO}$ and simulate optical properties of the structures under investigation. Optical properties are determined by transverse electromagnetic waves (in the terms of quantum mechanics, bulk plasmon phonon polaritons) excited in the structures under optical excitation. We simulate spectra of the complex permittivity, refractive index and extinction coefficient for bulk $n$-GaN considering contributions of free electrons and lattice vibrations. Then we calculate reflectivity and absorbivity spectra of the $n$-GaN/sapphire structures taking into account interference effects. Finally, we simulate the radiation emission spectra for various temperatures of the GaN epitaxial layer.

Experimental part of our work is devoted to reflectivity spectra measurements for the structures with various doping levels of GaN epitaxial layer. The experimental spectra are compared with the simulated ones. In the last section of the paper we summarize the major results.

2. Theoretical calculations

2.1. Plasmon–LO phonon modes in $n$-GaN

For a doped polar semiconductor, the dielectric permittivity at the angular frequency $\omega$ is given by [5, 6]:

$$
\varepsilon(\omega) = \varepsilon_\infty \left[ 1 + \frac{\omega_{LO}^2 - \omega_{TO}^2}{\omega_{TO}^2 - \omega^2 - i\omega\gamma} - \frac{\omega_p^2}{\omega^2 + i\omega\tau^{-1}} \right],
$$

where $\omega_{TO}$ is the frequency of a transverse optical (TO) phonon which is connected with the LO phonon frequency by the Lyddane–Sachs–Teller relation: $\varepsilon_0/\varepsilon_\infty = \omega_{LO}^2/\omega_{TO}^2$, $\varepsilon_0$ is the static permittivity, $\gamma$ is the damping constant for TO phonons, $\tau$ is the relaxation time determined by the mobility $\mu$ of electrons: $\tau = m_e\mu/e$.

Frequencies of the longitudinal electromagnetic waves which can propagate in a media can be found by solving the equation $\varepsilon(\omega) = 0$ [5] that gives two solutions for the doped polar semiconductor which are denoted below as $\omega_+^*$ and $\omega_-^*$. Generally, $\omega_+^*$ and $\omega_-^*$ are complex quantities. The real part of these quantities ($\omega_+ = \text{Re}\omega_+^*$ and $\omega_- = \text{Re}\omega_-^*$) gives the frequencies of plasmon–LO phonon modes. The imaginary part gives their decrements. It should be noted that there is no dispersion for the longitudinal electromagnetic waves in the long-wavelength limit where the wavevector $q \to 0$. Usually plasmon–LO phonon modes are detected by means of Raman spectroscopy. In particular, plasmon–LO phonon modes in $n$-GaN were experimentally studied in [7–9]. However, optical detection of these modes by means of reflectivity spectra is also possible. For low doped $n$-GaN ($N_e < 2 \times 10^{17}$ cm$^{-3}$), such investigations were carried out in [10].

In the present subsection we simulate plasmon–LO phonon modes in $n$-GaN in a wide concentration range taking into account the damping constant for TO phonons ($\gamma$) and the relaxation time for free electrons ($\tau$). In the next subsection we consider a correlation between the calculated frequencies of plasmon–LO phonon modes and peculiarities of the optical spectra (reflection and emission).
The concentration dependence of plasmon–LO phonon modes is presented in figure 1. To provide needed data on the dependence of $\tau$ upon $N_e$, we used the experimental dependence $\mu = \mu(N_e)$ obtained earlier on the basis of Hall measurements in $n$-GaN with various doping levels [11].

The simulation results based on these data are shown in figure 1 by green curves. The high frequency plasmon phonon mode $\omega_+$ at low concentrations is close to the LO phonon frequency $\omega_{LO}$ and at high concentrations is close to the plasma frequency $\omega_P$. The low frequency plasmon phonon mode $\omega_-$ at high concentrations is close to the TO phonon frequency $\omega_{TO}$. All three these limit values are the same as ones given by a simplified theory which does not take into account phonon damping and electron relaxation processes (that is equivalent to the case of $\gamma = 0$ and $\tau = \infty$ in equation 1). But in the case of $\tau \neq \infty$, the general theory (green lines in figure 1) gives a significantly different result for $\omega_-$ for low concentrations in comparison with the simplified theory (black lines in figure 1). While the simplified theory [6] gives $\omega_- = \omega_P - \sqrt{\frac{\varepsilon_\infty - \varepsilon_0}{\varepsilon_0}}$, the general theory considered here gives much less values.

Moreover, in accordance with our calculations, the low frequency plasmon phonon mode in $n$-GaN is completely overborne by electron scattering processes at concentrations $N_e < 1.8 \cdot 10^{17}$ cm$^{-3}$. It should be emphasized that both plasmon–LO phonon modes $\omega_+$ and $\omega_-$ can be located rather far from $\omega_P$ and $\omega_{LO}$ especially in the case of $\omega_P \approx \omega_{LO}$.

**Figure 1.** Concentration dependence of plasmon–LO phonon modes in $n$-GaN. Green lines: calculation taking into account the damping constant for TO phonons and the relaxation time for free electrons. Black solid lines: calculation for the collisionless electron plasma ($\tau = \infty$). Dotted lines denote electron concentrations in three samples under study.

### 2.2. Reflectivity and absorptivity spectra of $n$-GaN epitaxial layers

We simulate reflectivity and absorptivity spectra for $n$-GaN epitaxial layers grown on a sapphire substrate. We consider three values of electron concentration, namely, $N_e = 3.1 \cdot 10^{17}$, $5 \cdot 10^{18}$ and $3.6 \cdot 10^{19}$ cm$^{-3}$ (named as sample 1, sample 2 and sample 3) corresponding to three frequency ranges $\omega_P < \omega_{LO}$, $\omega_P \approx \omega_{LO}$, and $\omega_P > \omega_{LO}$, respectively.

Firstly, with the help of the Fresnel equation:
where we simulated spectra of the refractive index \( n \) and the extinction coefficient \( k \) for bulk \( n \)-GaN. In the calculations we used the following values of \( n \)-GaN parameters: \( \varepsilon_{\infty} = 5.4, \varepsilon_0 = 9.5, \hbar \omega_{\text{TO}} = 69.3 \text{ meV}, m_e = 0.2 m_0 [12, 13], \gamma = 2.4 \times 10^{11} \text{ s}^{-1}, \mu = 122 \text{ cm}^2/\text{V} \cdot \text{s} \).

**Figure 2.** Reflectivity (a), (b), (c) and absorptivity (d), (e), (f) spectra of \( n \)-GaN/sapphire structures under normal incidence of radiation (calculation).

Then we calculated the reflectivity \( R \) and transmittivity \( T \) spectra for different thicknesses of the epitaxial layer taking into account interference effects. Calculations were based on the analytical formulas from [14]. The value of the refractive index of the sapphire substrate was put as 2.9 [15]. In figure 2 we present the simulation results on the reflectivity of the GaN epilayer with the thickness of 6.2 \( \mu \text{m} \) under normal incidence of radiation.
One can see, that for the low-doped sample 1 (figure 2 (a)) the calculated reflectivity spectrum has a usual shape in the Reststrahlen band (in the spectral range between $\omega_{TO}$ and $\omega_{LO}$), and the plasmon phonon mode $\omega_p$ practically coincides with $\omega_{LO}$. The reflectivity $R$ has a deep minimum at the frequency $\omega \approx \omega_k \approx \omega_{LO}$. In the case of $\omega_P \approx \omega_{LO}$ (sample 2, figure 2 (b)), the reflectivity spectrum changes significantly and one can see two reflectivity minimums at the frequencies of plasmon phonon modes $\omega_-$ and $\omega_+$. Finally, in the case of the heavily doped sample 3 (figure 2 (c), the superposition of the Reststrahlen band and plasma reflection band takes place at frequencies $\omega \leq \omega_{LO}$ and one can see a very unusual sharp dip in the reflectivity spectrum at $\omega \approx \omega_- \approx \omega_{LO}$ and the second reflectivity minimum at $\omega \approx \omega_+ \approx \omega_P$. Thus, analysis of the calculated reflectivity spectra shows that the reflectivity minimums are always very close to the frequencies of the plasmon phonon mode $\omega_-$ and $\omega_+$. There is one exception only: in the low-doped sample with low electron mobility the reflectivity minimum $\omega \approx \omega_k$ is inexpressive.

Using the data on the calculated transmittivity of the GaN/sapphire structures under normal incidence of radiation, we then determined absorptivity spectra with the help of the equation $A = 1 - T - R$. The results of simulation for all three samples are presented in figure 2 (d), (e), (f). Analysis of the calculated absorptivity spectra shows that they are characterized by the intensive absorption lines at the frequencies of the plasmon phonon mode $\omega_-$ and $\omega_+$. These absorption lines are especially well pronounced in cases of $\omega_P \approx \omega_{LO}$ and $\omega_P > \omega_{LO}$ (figure 2 (e) and (f)). In the latter case, the absorption line at $\omega \approx \omega_+ \approx \omega_{TO}$ represents a very sharp resonance.

It should be noted that in addition to abovementioned peculiarities, the reflectivity and absorptivity oscillate according to the frequency in the spectral ranges where the epitaxial layer is transparent enough. These oscillations are caused by the interference of electromagnetic waves in the epitaxial layer.

3. Experimental results and their discussion

Wurtzite gallium nitride epitaxial layers doped with silicon were grown by MOVPE on a $c$-plane sapphire substrate covered by a 2 $\mu$m undoped GaN buffer layer. Two structures were grown. In one structure $n$-GaN epitaxial layer is characterized by the following parameters: thickness $d = 10 \mu$m, electron concentration $N_e = 5 \times 10^{18}$ cm$^{-3}$ and mobility $\mu = 189$ cm$^2$/V·s (sample 2). The other structure contains a heavily doped $n$-GaN epilayer: $d = 6.2 \mu$m, $N_e = 3.6 \times 10^{19}$ cm$^{-3}$, $\mu = 122$ cm$^2$/V·s (sample 3). The concentration and mobility were determined by means of Hall and conductivity measurements at room temperature. It is known that at such doping levels GaN demonstrates formation of an impurity band [11] and free carriers are not frozen even at liquid helium temperatures.

The reflectivity spectra were investigated at room temperature using a Fourier spectrometer and a pyroelectric detector in the spectral range 8–80 meV (2–20 THz). A globar and a mercury lamp were used as sources of radiation. The incidence angle $\theta$ was about 11°, reflectivity measurements were carried out with an angular aperture of $\Delta \theta = 16^\circ$. An aluminum mirror was used as the reflectivity reference.

Experimental reflectivity spectra demonstrate the same peculiarities as were predicted by theoretical simulation (figure 2 (b), (c)). Because it is difficult to determine the exact value of the reference mirror reflectivity, we normalized the experimental spectra to the local maximum of reflectivity in the vicinity of $\omega_{TO}$. The normalized experimental reflectivity spectra are presented in figure 3 by black lines. The theoretical spectra were normalized by the same manner and were fitted to the experimental ones. Three quantities, namely $N_e$, $\mu$ and $\gamma$, were used as fitting parameters. The theoretical reflectivity spectra at the optimum values of the fitting parameters ($N_e'$, $\mu'$ and $\gamma'$) are shown in figure 3 by red lines. There is a good agreement between the experimental and theoretical spectra.
for both samples. In particular, both spectra demonstrate a local reflectivity minimum in the close vicinity of the frequency of plasmon polariton mode $\hbar \omega_p$ (figure 3 (a), (b)).

![Figure 3](image.png)

**Figure 3.** Normalized reflectivity spectra of the samples 2 and 3: experiment (black curves) and theoretical fit (red curves). Dotted lines denote the spectral position of the low frequency plasmon phonon mode $\hbar \omega_p$.

It should be noted that the values of the electron concentration and mobility obtained from the reflectivity spectra ($N_e' = 2.8 \cdot 10^{18} \text{ cm}^{-3}$ and $\mu' = 180 \text{ cm}^2/\text{V}\cdot\text{s}$ for the sample 2, $N_e' = 1.9 \cdot 10^{19} \text{ cm}^{-3}$ and $\mu' = 179 \text{ cm}^2/\text{V}\cdot\text{s}$) differ slightly from the values determined by Hall measurements. The latter are related to the average values across the whole GaN layer, but the former characterize only a subsurface region of the layer. The value of the damping constant for TO phonons ($\gamma'$) obtained from the reflectivity spectra is $7.5 \cdot 10^{11} \text{ s}^{-1}$. Thus, study of the reflectivity spectra is an effective method of contactless determination of electron concentration, mobility and TO phonon damping constant of n-GaN epitaxial layers.

4. Expected emission spectra
In the section 3 it was demonstrated that the reflectivity spectra considered in section 2 fit well the experimental results on radiation reflection for the samples 2 and 3. It is reasonable to suppose that the simulated absorptivity spectra for these samples (see figure 2 (e), (f)) will describe well the radiation absorption in the samples. In accordance with Kirchhoff’s law, for a body at thermal equilibrium the emissivity is equal to the absorptivity. That is why one can describe blackbody-like emission of the considered samples by means of Planck theory. The spectral density of radiation emission from an n-GaN epitaxial layer in the direction perpendicular to the sample surface in the limits of solid angle $\Omega << 2\pi$ is given by:

$$D(\omega, T) = \frac{\hbar \omega^3}{4\pi^2 c^2} \cdot A(\omega) \cdot \left[ \exp \left( \frac{\hbar \omega}{k_B T} \right) - 1 \right] \cdot \Omega,$$

where $T$ is the temperature of the n-GaN epitaxial layer, $k_B$ is the Boltzmann constant, $c$ is the light velocity.

Figure 4 demonstrates the simulation results on the spectral dependencies of $D$ for the samples 2 and 3 at different temperatures $T$. In every sample at high enough temperature one can see two
selective emission bands in the mid infrared range in the vicinity of plasmon phonon modes $\omega_-$ and $\omega_+$. The emission band in the vicinity of $\omega_-$ is much narrower than the one in the vicinity of $\omega_+$. The increase of electron concentration results in a "blue" shift of both emission bands. There is an opportunity to modulate the epilayer temperature by means of electric current, for instance, applying periodical pulses of electric voltage. This allows to develop emitters of modulated mid infrared radiation.

![Figure 4](image-url)

**Figure 4.** Dependence of the spectral density of radiation emission on photon energy. Theoretical simulation for the samples 2 (a) and 3 (b) at different temperatures. The solid angle $\Omega = 0.043$ sr corresponds to an angular aperture $\Delta \theta = 16^\circ$.

5. Conclusions
Transverse and longitudinal electromagnetic waves in $n$-GaN epitaxial layers have been studied theoretically and experimentally. Epitaxial layers with electron concentration in the range $10^{17} – 10^{19}$ cm$^{-3}$ have been examined. Simulation of the reflectivity and absorptivity spectra has been performed in the terahertz and mid infrared spectral ranges (the angular frequency range of $10^{13} – 10^{15}$ s$^{-1}$). Additionally, the radiation emission spectra have been simulated for various temperatures of the GaN epitaxial layer. It has been shown that the resonance peculiarities of the optical spectra are located closely to the frequencies of the coupled plasmon phonon modes. Experimental studies of the reflectivity spectra have been performed in the spectral range 8–80 meV (2–20 THz). The experimental spectra are well fitted by the simulated ones and can be used for contactless determination of the electron concentration, mobility and TO phonon damping constant in GaN epitaxial layers. The experimental and theoretical results of the present work provide insights for the development of GaN-based devices aimed to absorb/emit terahertz or mid infrared radiation selectively. In particular, electrically controlled emitters of modulated mid infrared radiation can be developed.

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