Modulation Intersubband Absorption and the Hot Electron Mechanism in Heterostructure of Al$_{1-y}$In$_y$N/Ga$_{1-x}$In$_x$N

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We have theoretically investigated the modulation of the intersubband absorption coefficient of the heterostructure of Al$_{1-y}$In$_y$N/Ga$_{1-x}$In$_x$N with an optimum well width of 1.5 nm. The value of the intersubband absorption coefficient increased significantly as a function of the electric field applied. The scattering energy rate between electrons and LO phonons as a function of the hot electron temperature, taking into account the non-equilibrium optical phonon accumulation model, is lower than without taking this model into account. The models of the modulation of the intersubband absorption were studied when the effect of the non-equilibrium optical phonon accumulation as a function of the applied electric field was taken into account, and also when this effect was not taken into account. Due to the changing rate of the optical phonons with the wave vector $q$, the modulation of the intersubband absorption with non-equilibrium optical phonon accumulation was higher than that without non-equilibrium optical phonon accumulation.

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I. INTRODUCTION

In recent years, several papers have been published about optical phenomena in quantum wells (QW) with regard to the fabrication of a mid-IR and terahertz range laser. The papers suggested, for example, that the design and properties of nanostructures strongly supported the intersubband population inversion between two excited states of electron energy levels in QWs under both current and optical pumping [1–4]. Those nanostructures mostly were based on III-V compound semiconductor heterostructures. One of the most challenging structures is the heterostructure deposited on III-nitride semiconductors, especially GaN. GaN-based semiconductors have special characteristics. For example, there are two types of crystalline structures, wurtzite and zincblende, with energy band gaps of 3.2 eV and 3.39 eV, respectively, and both exhibit stability under high temperatures and strong electric fields. Wurtzite, especially, has a significant potential for electronics and optical applications. Several research papers have been published in recent years about optoelectronics devices based on nanostructures deposited on wurtzite GaN substrates. These researches have studied the intersubband electron transitions in the quantum wells and
their relevance to a quantum cascade laser (QCL) for telecommunication applications [5], modulators in the UV range [6], and other optoelectronics devices [7]. When considering intersubband electron transitions at telecommunication wavelengths between 1.3 and 1.55 µm for a QCL, the design of the heterostructure of the AlN deposited on the GaN substrate must be selectively considered. From Vegard’s law [8, 9] the width of the quantum wells of the heterostructures can determine the energy band gap and lattice constant, and, correspondingly, the electron energy levels in quantum wells can, in principle, be controlled. As a result, the required intersubband transition wavelength can be reached. Nevertheless, because of the structural defect due to the lattice mismatch of the AlN/GaN heterostructure, the structure must be designed in order to minimize as much as possible the structural defects during the growing process. Therefore, we referred to the strain-free Al$_{1-y}$In$_y$N/Ga$_{1-x}$In$_x$N ($y = 17.7\%$, $x = 0$) quantum well structures grown on the wurzite GaN substrate studied in [10], with a lattice constant close to $a_{\text{GaN}}$ and with intersubband transition wavelengths suitable for telecommunications; the electron transition energy in the active region produced a wavelength of around 2 µm. The purpose of this paper is to study, using the principle of hot charge carriers phenomena, the change in the intersubband absorption coefficient, which theoretically relates to the intersubband transition energy between two energy levels of electrons in a nanostructure from the referenced paper [10]. The study of the hot electron phenomena is one of the techniques to improve devices’ performance, since these phenomena can induce a change in the physical properties of subsystems [11–15]. These phenomena can be explained by the influence of either a high optical pumping intensity or strong electric field on the nanostructures, inducing carriers to have higher kinetic energy, hence influencing the lattice temperature and, consequently, the carriers’ temperature. These carriers with increased kinetic energy must conserve this excess energy, transferring it to the whole subsystem by scattering to other particles or quasi-particles: polar optical phonons or acoustical phonons. In order to improve the inversion population condition of the quantum cascade laser (QCL), the intersubband absorption coefficient relating to the intersubband transition energy of the electrons in the quantum wells must increase. Moreover, it is necessary to discover a way to reduce the scattering rate of carriers at the structural defects of the GaN substrate to support the higher electron transition energy, which is necessary to improve the performance of the QCL. In order to execute this mission, research into the carriers’ scattering energy rate must be theoretically conducted. The consideration of non-equilibrium LO phonon accumulation significantly decreased the carriers’ scattering energy rate in the subsystem [16–18]. As a result, the electron transition energy and, consequently, the inversion population of electrons, which is one of the most important of laser properties, will be significantly increased.

II. MATERIALS AND METHODS

In this research, we theoretically studied the change in the intersubband absorption coefficient brought about by the application of a lateral electric field and the hot electron mechanism in Al$_{1-y}$In$_y$N/Ga$_{1-x}$In$_x$N structures deposited on a wurzite GaN substrate with
a lattice constant close to \( a_{\text{GaN}} \). This studied structure was published in [10]. From that research, the optimum width of the quantum well was 1.5 nm, while the width of the barrier was 2 nm and the quantum well structure had two confined electron energy levels. By solving the Schrödinger equation together with the Poisson equation one can determine the wave functions and the energy spectrum of the electronic states (the energy spectrum and wave functions of this structure were presented in the referenced article [10]).

III. RESULTS AND DISCUSSION

III-1. The calculation of the equilibrium intersubband absorption coefficient

With this specification of the electron energy levels, the calculation of the equilibrium intersubband absorption coefficient can be obtained from the intersubband transition probability from the initial state of subband \( i \) to the final state of subband \( j (e_i \rightarrow e_j) \) in the quantum well. From Fermi’s golden rule [19], it is given by

\[
W_{fi} = \frac{2\pi}{\hbar} |V_{fi}|^2 \delta (\varepsilon_f - \varepsilon_i),
\]

(1)

\[
\varepsilon_i = \varepsilon_{0i} + \frac{\hbar^2 k_i^2}{2m_i}, \quad \varepsilon_f = \varepsilon_{0f} + \frac{\hbar^2 k_f^2}{2m_f},
\]

(2)

\( \varepsilon_i \) and \( \varepsilon_f \) are, respectively, the total energy of the initial and final states of the subbands, and \( \varepsilon_{0i}, \varepsilon_{0f} \) are the minimum energy levels of the subbands \( e_i \) and \( e_f \),

where \( V = \int \psi_f^* \hat{V} \psi_i d\Omega = \langle \psi_f | \hat{V} | \psi_i \rangle \)

(3)

is the matrix element

and \( \hat{V} = \frac{e}{m_0} \left( \frac{2\pi \hbar N_\omega}{\Omega \chi \omega} \right)^{1/2} \vec{e}_\omega \cdot \vec{p} \)

(4)

is the operator of the interaction energy between the electrons and photons, \( N_\omega \) = the number of photons, \( \Omega \) = volume of unit cell, \( \vec{e}_\omega \) = the unit vector of light polarization, \( \vec{p} = -i\hbar \nabla \) is the momentum operator, \( \chi \) = the high frequency dielectric constant of GaN (assuming that the refractive indices of the well and barrier materials are similar) and \( m_0 \) = the mass of a free electron.

For z-polarized light of frequency (\( \omega \)) and electron transition between the initial and final states of the subband, the absorption coefficient \( \alpha_{fi}(\omega) \) can be determined from perturbation theory [20]. Therefore from this theory the intersubband transition probability in the QW and the intersubband absorption coefficient are related to each other thus:

\[
\alpha_{fi}(\omega) \propto \sum_{i,f} W_{fi} [f(\varepsilon_i) - f(\varepsilon_f)],
\]

(5)
or in another way:

$$\alpha_{fi}(\omega) \propto \sum_{i,f} |V_{fi}|^2 \cdot \delta(\epsilon_f - \epsilon_i - \hbar \omega)[f(\epsilon_i) - f(\epsilon_f)]. \quad (6)$$

Then, from (1) and (4) above, we obtained:

$$\alpha_{fi}(\omega) = \frac{4\pi^2 e^2 N\omega}{\Omega \chi \omega m_0^2} \times \sum_{k_i} \sum_{k_f} \left| e_z \delta_{k_i,k_f} \int \psi_f^*(z) \hat{p}_z \psi_i(z) dz \right|^2 \times [f_i(\epsilon_i) - f_f(\epsilon_f)] \delta[\epsilon_f - \epsilon_i - \hbar \omega], \quad (7)$$

where $f(\epsilon_i)$ and $f(\epsilon_f)$ are the Fermi-Dirac distribution functions of the electrons on the initial and final states of the subband, respectively; $k_i$ and $k_f$ are the two dimensional wave vectors of electrons in the initial and final states of the subband, respectively, and $e_z$ is the $z$-component of the vector polarization of light. The $z$-component of the momentum operator, $\hat{p}_z$ and its matrix element can be written in terms of the dipole moment of transition ($\hat{p}_z$)$_{fi} = i\omega m_0 z_{fi}$, where $z_{fi} = \int \psi_f^*(z)z\psi_i(z)dz$, which is the optical matrix element of the $z$ co-ordinate describing the probabilities of the intersubband optical transition $e_i \rightarrow e_f$. Substitute this into (7) and apply an integral instead of summation and then the absorption coefficient for the optical transition of $e_1 \rightarrow e_2$ will be obtained as

$$\alpha_{21}(\omega) = \frac{4\pi^2 e^2 \omega^2 N\omega}{\Omega \chi \omega \cos^2 \theta_{21}^2} \times \int \frac{2S}{(2\pi)^2} \left[f_1(\epsilon_1) - f_2(\epsilon_2)\right] \delta[\epsilon_2 - \epsilon_1 - \hbar \omega] dk, \quad (8)$$

where $S$ is the area of the structure. For the optimum well width of 1.5 nm, the equilibrium intersubband absorption spectrum, shown as light dots, obtained from this equation is presented in Fig. 1.

III-2. The calculation of the modulation intersubband absorption coefficient

To increase the electron concentration in the subband level 1 ($e_1$) and, thus, correspondingly influence the change in the intersubband absorption coefficient, we need to consider the energy spacing between level 1 and level 2 ($\Delta_{21}$). The electron energy spacing between subband levels 1 and 2, the optical matrix element $z_{21}$, the chemical potential ($\mu$) and the electron concentrations on subband levels 1 and 2 are all functions of the lattice temperature [21]. These properties can determine the behavior of the absorption coefficient. To improve the intersubband electron transition probabilities between the electron energy subband 1 and subband 2 and, thus, the intersubband absorption coefficient, the application of an electric field to the structure was theoretically considered. The spectrum of the absorption coefficient ($\alpha_{21}$) compared with the modulated coefficient ($\Delta\alpha_{21}$) obtained theoretically by the application of an electric field of 1000 V/cm is presented in Fig.1,(the method of this calculation was presented for example in [21] and [22]). A strong electric field applied to nanostructures induces the carriers to have higher kinetic energy, influencing the lattice temperatures and consequently the carriers’ temperatures. These carriers, the hot electrons, conserve this excess kinetic energy by transferring it to the whole system
FIG. 1: The equilibrium absorption coefficient spectrum for the optical transition of $e_1 \rightarrow e_2(\alpha_{21})$ compared with the absorption coefficient for the optical transition of $e_1 \rightarrow e_2$ under application of an electric field of 1000 V/cm ($\Delta \alpha_{21}$).

through scattering to other particles or quasi-particles, for example, polar longitudinal optical (LO) phonons or deformational acoustic (DA) phonons. In semiconductors based on III-nitride, the carrier scattering process involves the emission of LO phonons. An energy balance equation (EBE) in this case can determine the carrier scattering rate [13].

$$e \mu_n E^2 = \left\langle \frac{d\varepsilon}{dt} \right\rangle_{LO},$$

where $e$ is the electron free charge, $\mu_n$ is the mobility of electrons, and $E$ is the applied electric field.

The left side of (9) explains the collecting energy rate of electrons from the system. In equilibrium conditions, it must equal the transferring energy rate of electrons to the lattice and thus the carriers’ scattering energy rate, which is averaged for all the electrons in the system (the right side of (9)).

To reduce the carrier scattering energy rate of electrons in subbands, the non-equilibrium optical phonon accumulation model must be taken into account.

The distribution function of non-equilibrium optical phonons can be written as

$$N^q = N^0_q + \frac{dN^q_q}{dt} \tau_{q, LO},$$

where $N^0_q = [\exp\left(\frac{E_{ph}}{k_B T}\right) - 1]^{-1}$ is the distribution function of the equilibrium optical phonons, $k_B$ is Boltzmann’s constant, $T$ is the lattice temperature, $\tau_{q, LO}$ is the optical phonon lifetime, and $\frac{dN^q_q}{dt}$ is the changing rate of optical phonons with phonon wave vector.
The changing rate of optical phonons can be calculated by perturbation theory with the matrix element of the interaction between the optical phonons and electrons in the system. Consequently, the energy balance equation can be written as

\[ e \mu_N E^2 = \left\langle \frac{d\varepsilon}{dt} \right\rangle_{LO} = \sum_q \hbar \omega_0 \frac{dN_q}{dt}, \]  

(11)

where \( \hbar \omega_0 = 90 \text{ meV} \), which is the LO phonon energy value for GaN. The summation sign is calculated for all optical phonon wave vectors in unit cells. The results of the calculation of the carriers’ scattering energy rate using the non-equilibrium phonon accumulation model refer to a calculation model in \[22, 23\] applied to the structure studied here and presented in Fig. 2 (dark spots). For this structure, we used a polar optical phonon lifetime \( \tau_{q;LO} = 5 \cdot 10^{-12} \text{ s} \) \[24\]. The accumulation of non-equilibrium polar optical phonons depends on the polar optical phonon lifetime \( \tau_{q;LO} \). Therefore, as shown in Fig. 2, compared with the results achieved without including the calculation of the non-equilibrium phonon accumulation effect (the solid line), the results achieved including calculation of that effect indicate a lower carrier scattering energy rate from the same structure.

FIG. 2: Carrier scattering energy rate of 2D electrons scattering with a polar optical phonon as a function of the hot electron temperature of the QW.

From (9) and (11) with the optical phonon lifetime \( (\tau_{q,LO}) \) of \( 5 \cdot 10^{-12} \text{ s} \) for the GaN wurtzite structure, the change in the intersubband absorption coefficient as a function of the applied electric field is presented in Fig. 3. Comparing the results attained with and without the non-equilibrium phonon accumulation effect: the change in the intersubband absorption coefficient with non-equilibrium phonon accumulation (solid line) is significantly higher with an increase of the applied electric field. We submit that the distribution function
for non-equilibrium optical phonons, as a function of the changing rate of optical phonons with phonon wave vector \( q \), indicates a slowing down of the energy relaxation process between the electrons and phonons at the electron energy subband 1. Therefore, with an increase in the strength of the applied electric field, the electron concentration on subband 1 will be increased, and at the same time the relaxation process will slow down with the accumulation of optical phonons.

![Image](image_url)

**FIG. 3:** The dependence of the change in the intersubband absorption coefficient on an applied electric field at the electron transition energy of 650 meV [10] with (bold line) and without (broken line) the non-equilibrium optical phonon accumulation effect.

In principle, the energy relaxation rate (or carrier scattering energy rate) of the electrons in energy subband 1 and subband 2 can be different, since the electron wave function on both subbands can exist in different forms and locations. As a result, from the EBE (9) and (11), the electron mobility of each subband can also be different, as can the hot electron temperature. Since the electron mobility is a function of the carriers’ scattering energy rate and the changing rate of optical phonons, the EBE can be written as:

\[
\frac{dN_q}{dt} = \varphi(T_e, \tau_{q,LO}),
\]

\[
e\mu_n E^2 = \left\langle \frac{d\varepsilon}{dt} \right\rangle_{LO} = \sum_q \hbar \omega_0 \frac{dN_q}{dt} = \sum_q \hbar \omega_0 \varphi(T_e, \tau_{q,LO}).
\]

From (12) and (13), with optical phonon lifetime (\( \tau_{q,LO} \)), the hot electron temperature (\( T_e \)) can be determined as a function of the applied electric field as well as the energy spacing between subband 1 and subband 2. Our next investigation will look at different well widths.
for this heterostructure \((\text{Al}_{1-y}\text{In}_y\text{N/Ga}_{1-x}\text{In}_x\text{N})\) with less lattice mismatch. Since the well width of the quantum well, energy band gap and lattice constant of a heterostructure relate to each other according to Vegard’s Law, the electron energy levels in a quantum well, and consequently the intersubband transition energy of electrons, can be optimally controlled.

To improve the performance of a quantum cascade laser (QCL), the number of subband levels should be selectively considered [24], so that the inversion population of electrons on the electron energy levels can be most effectively accomplished.

**IV. CONCLUSION**

In this paper, we theoretically investigated the modulation of the intersubband absorption coefficient of a heterostructure of \(\text{Al}_{1-y}\text{In}_y\text{N/Ga}_{1-x}\text{In}_x\text{N}\) with the optimum well width of 1.5 nm. This kind of structure has two confined electron energy levels in its quantum well. To obtain the change in the intersubband absorption coefficient between subband 1 and subband 2, an electric field of 1000 V/cm was theoretically applied. As a result, the equilibrium intersubband absorption coefficient was modulated. With the application of a strong electric field, the electrons in the structure obtained excess energy and a higher temperature. These high-energy electrons have to transfer this excess energy to the system by the scattering process with the emission of polar longitudinal optical phonons (LO phonons). To slow down this scattering process, the non-equilibrium optical phonon accumulation model was taken into account. This model was proposed to consider the change in the distribution function of non-equilibrium optical phonons. Due to the changing rate of optical phonons with phonon wave vector \(q\), from the energy balance equation, the change in the intersubband absorption coefficient was greater when we used the non-equilibrium optical phonon accumulation model than it was if we did not use this model.

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