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PHONON SPECTRUM OF LED InGaN/GaN HETEROSTRUCTURE WITH QUANTUM WELLS

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The measurements of the phonon spectrum of a LED heterostructure based on the $In_{0.12}Ga_{0.88}N/GaN$ *barrier showed the presence of four phonon radiation peaks with energies of 0.193, 0.207, 0.353, and 0.356 eV. It was assumed from the comparison of the calculation results of energy spectra of the electron and hole quantum wells with the obtained experimental data that these peaks can be interpreted as the energies of phonons generated during the capture of electrons from the barrier layer to the second level of dimensional quantization, as well as during the relaxation of electrons from the second level to the radiation level and trapping of holes to the upper level of the quantum well.*

Keywords: quantum well, electron capture, phonons, spectrum, Kubelka–Munk transformations

INTRODUCTION

Currently, insufficient attention is paid in the scientific literature to the consideration of the capture and emission mechanisms of charge carriers by a quantum well (QW) in LED heterostructures (HSs). In turn, these mechanisms set the injection current in the QW, which determines the efficiency of a LED HS. There are several models describing the capture and emission of charge carriers to energy levels: the J. Thomson model [1], the Lax cascade model [2], the Abakumov–Perel model [3, 4], and the Shockley–Reed–Hall model [5–7]. However, until now, none of them takes into account (in the volume required for the agreement with the experiment) the fundamental features of the QW and charge carriers interaction associated with the participation in the resonance capture – the emission of free electrons and phonons with the formation of a standing wave with a difference energy representing the spectrum of an electron in the QW [3, 4, 8–10].

INITIAL POSITIONS

The energy diagram of the electron (n-QW) and hole (p-QW) quantum wells (Fig. 1) shows that the process of interaction between the charge carriers and a QW consists in the capture of a carrier to the upper level of dimensional quantization (DQL) with a characteristic time $\tau_{cap}^{(n)}$ or in its emission with the time $\tau_{em}^{(n)}$ [10]. The excess energy of the captured electron and hole is realized in the form of phonons with the energies $E_{ph1}^{(n)}$ and $E_{ph1}^{(p)}$, respectively. Emission of several phonons with different energies is possible, but one-phonon processes are apparently more probable.

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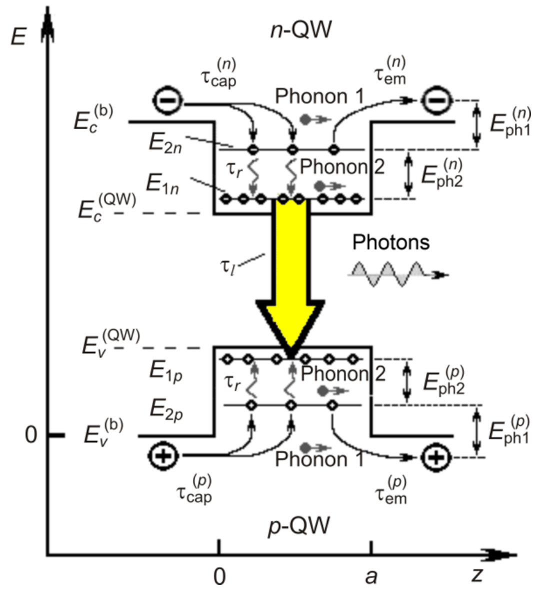

Fig. 1. Capture and emission of charge carriers by QW with phonon generation.

Then, the captured carriers relax to the lower levels $E_{1n,p}$ after the time τ_r with the emission of phonons of the difference energies $E_{ph2}^{(n)}$ and $E_{ph2}^{(p)}$, from which radiative band-to-band transitions with the recombination time τ_l occur.

It follows from the analysis of interaction of free charge carriers with QWs, that the ratios of the times of capture, emission, nonradiative relaxation and the time of radiative recombination are decisive for obtaining a high internal quantum yield of radiation emission: the characteristic times $\tau_{em}^{(n)}$ and $\tau_{em}^{(p)}$ should be maximum, while the characteristic times $\tau_{cap}^{(n)}$, $\tau_{cap}^{(p)}$, τ_r, and τ_l should be minimal.

The descriptions of the free electron state in the barrier layer and of an electron-wave in the quantum well do not cause difficulties. However, the description of the third participant of the interaction – an optical or acoustic phonon in a QW – requires a separate consideration. At present, there are not enough works in the literature on the study of physical processes of the phonon spectra formation in QWs consisting of InGaN and the GaN – InGaN interface. The available data indicate that optical phonons are the main participants of the process of capture of charge carriers in QWs [11–13]. However, there is no data on the phonon formation mechanism and on the numerical values of the phonon energies as applied to the capture of electrons and holes in heterostructures based on the $In_{0.12}Ga_{0.88}N$ compound widely used in practice.

The aim of this work is an experimental study of the phonon spectrum of a LED HS with QWs to reveal its basic structure and features in the light emission mode, as well as the frequencies of optical phonons responsible for the capture of carriers in QWs.

EXPERIMENTAL

The samples under study were light-emitting heterostructures based on $In_{0.12}GaN/GaN$ barriers, in which there was no luminophore layer at the radiation output. Their phonon spectra were measured by the Fourier transform spectroscopy [14] by recording the diffuse reflectance spectra in the range 0.04–0.5 eV (400–4000 cm^{-1}) on a Shimadzu IRTracer-100 Fourier Transform Infrared Spectrophotometer (FTIS) with a DRS-8000A box [14]. Coherent radiation

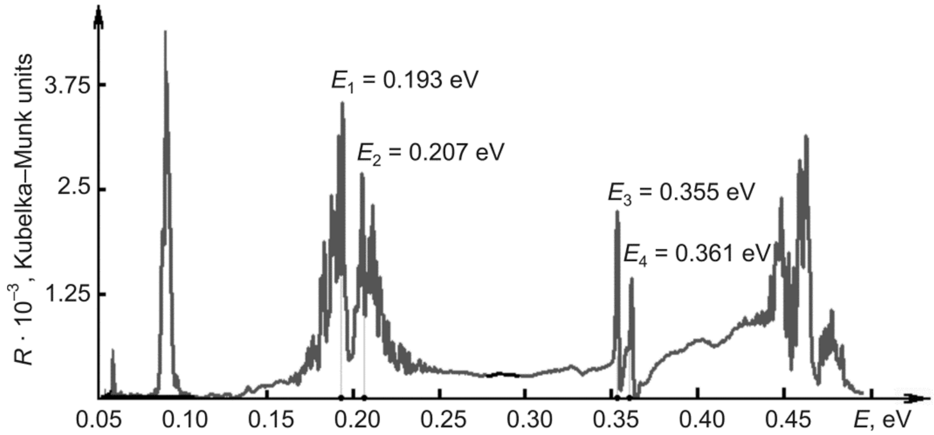

Fig. 2. Phonon spectrum of the emitting InGaN/GaN heterostructure. The spectrum of the switched off heterostructure is subtracted.

from the red region of the visible spectrum was used to excite the nonequilibrium state of the samples. In the experiments performed, about a dozen heterostructures were investigated, which showed qualitatively the same results.

Along with the recording the diffuse reflection spectra of LED heterostructures, the phonon spectra of the diffusion gallium arsenide AL106 LEDs with a red emission line were measured in the experiment. Comparison of the spectra of the diffusion LEDs and LED HSs makes it possible, with a certain degree of certainty, to select the regions of the HS spectrum, absent in the spectra of the diffusion LEDs, which contain information on the interaction of charge carriers with the phonons in the QW.

To exclude the systematic error, at the beginning of the experiment, the spectrum of the switched off HS was measured, which was considered as the background. Then, the spectrum of the switched on HS was recorded, from which the background spectrum was subtracted. The resulting spectrum was considered final. In the LabSolutions IR software operating with the Shimadzu IRTracer-100 FTIS, the difference diffuse reflectance spectra obtained using the Kubelka–Munk transformation were converted into the absorption spectra of the object under study [15, 16].

EXPERIMENTAL RESULTS

The shape of the HS long-wavelength reflection absorption spectrum (RAS) in the visible range is shown in Fig. 2. Its comparison with the phonon spectrum of a diffusion LED showed that their difference is caused by the existence in the spectrum of LED HS of two regions of the reflection absorption coefficient peaks with energies in the ranges of 0.18–0.22 eV and 0.35–0.36 eV. Their presence is considered as a result of the effect of QWs on the generation of optical radiation with the formation of phonons in the HS. In the RAS of the switched on HS, many peaks of long-wave radiation were also detected. The most significant peak with an energy of 0.09 eV can be associated with the longitudinal optical phonons [17]. The peaks in the range of 0.45–0.48 eV are probably associated with the water-containing compounds.

Considering the obtained results of measuring the phonon spectrum from the standpoint of the classical Lorentz model in the framework of one-phonon resonance [14], the indicated energies can, with a high degree of probability, be associated with the energies of phonons formed in the HS upon emission of visible light. This is the energy that an electron gives to the QW substance lattice under transition from the conduction band of the barrier to the upper DQL of the well. For a typical *n*-QW depth in LED heterostructures equal to 0.40 eV and an indium fraction in the well composition equal to $x = 0.12$ in the 1.9 nm thick $In_{0.12}Ga_{0.88}N$ QW, there will be only two DQLs with energies of $E_{1n} \approx 0.06$ eV and $E_{2n} \approx 0.24$ eV. Then, the capture of an electron to the upper level will be accompanied by the release of an excess energy $E_{\text{ph1}}^{(n)} \approx 1.8kT + \Delta E_c - E_{2n} \approx 0.05 + 0.40 - 0.24 = 0.21$ eV. This energy value of the emitted phonon is close to the energy of the phonon spectrum peak $E_2 = 0.207$ eV.

Another channel of phonon generation in LED HSs is the relaxation of captured electrons from the upper level to the lower radiative level. The energy released in this case is equal to the difference between the energies of the upper and lower DQLs: $E_{\text{ph2}}^{(n)} = E_{2n} - E_{1n} = 0.24 - 0.06 = 0.18$ eV, which, within the experimental accuracy, falls into the region of the phonon spectrum peak $E_1 = 0.193$ eV (Fig. 2).

The second peak of the phonon density with an energy of 0.18 eV is probably caused by the capture of a hole by the DQL in the hole well. Due to the difference in the effective masses of electrons m_n^* and heavy holes m_p^* in $In_{0.12}Ga_{0.88}N$, the energy spectrum for holes is $E_{kp} = E_{kn}\left(m_n^*/m_p^*\right)$ times denser than that for electrons. Then, the DQLs in the p-QW will have the following energies:

$$E_{1p} = E_{1n}\left(m_n^*/m_p^*\right) = 0.06\left(0.189m_0/0.90m_0\right) \approx 0.01 \text{ eV}, \quad E_{2p} = E_{2n}\left(m_n^*/m_p^*\right) \approx 0.05 \text{ eV}.$$

At a p-QW depth of $\Delta E_v = 0.24$ eV, the capture of holes to the level E_{2p} will be accompanied by the emission of a phonon with an energy of 0.18 eV, which can be interpreted as the second peak in the phonon spectrum. The numerical values of the parameters of the heterostructure with InGaN QWs correspond to the parameters of real heterostructures [18, 19].

Note that the relaxation of a captured hole to the radiative level will be accompanied by the emission of phonons, whose energy is outside the discussed peaks.

CONCLUSIONS

From the experimentally measured RAS of a LED HS with QWs based on the InGaN/GaN barrier, as well as the spectra of a diffusion LED, the spectra of a light-emitting HS with QWs were calculated. The obtained spectra revealed two ranges of phonon frequencies (0.18–0.22 eV and 0.35–0.36 eV) associated with the features of the process of free charge carriers capture by the electron and hole quantum wells.

The calculations show that for HSs with the QW thickness of $a \approx 1.9$ nm and an In content in the cation sublattice of 12%, typical for LED sources, phonons with an energy of $E_2 = 0.207$ eV are probably formed as a result of the electron capture from the barrier to the second DQL in the electron well: $E_{\text{ph1}}^{(n)} = E_2$. The subsequent relaxation of electrons to the lower level is accompanied by the generation of phonons with the energy $E_{\text{ph2}}^{(n)} = 0.18$ eV, which, due to the broadening of the spectrum and the approximate calculation of the DQL, can be identified with the phonon density peak $E_1 = 0.193$ eV: $E_{\text{ph2}}^{(n)} \approx E_1$. The phonons emitted during the capture of holes by the second DQL have the same energy $E_{\text{ph1}}^{(p)} \approx E_1$.

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