Non-equilibrium hole capture to excited acceptor states in quantum wells due to optical scattering

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Abstract. The probability of optical-phonon-assisted scattering of non-equilibrium holes to excited acceptor states in GaAs/AlGaAs quantum wells is considered. In the model we used, a well-known expression for the probability of intersubband optical scattering of two-dimensional carriers was expanded to the case when the final hole state is the excited state of an acceptor center. The temperature dependences of the probability of hole capture to excited acceptor states with simultaneous optical phonon emission are calculated. The result allows one to estimate the contribution of optical scattering to the experimentally observed terahertz electroluminescence due to intracenter carrier transitions.

1. Introduction
The binding energies of shallow impurities in doped semiconductors and semiconductor nanostructures correspond to the terahertz (THz) spectral range. Currently, the terahertz radiation emission associated with the radiative capture of non-equilibrium carriers on impurity centers in doped quantum well (QW) structures is extensively investigated. Terahertz photoluminescence associated with donor states was experimentally observed in $n$-GaAs/AlGaAs QWs [1] under interband optical excitation in the case of both spontaneous and stimulated near-IR luminescence due to transitions from the ground donor state to the valence band. Low-temperature terahertz electroluminescence of acceptors in $p$-GaAs/AlGaAs QWs under conditions of impurity breakdown in a strong lateral electric field was reported in [2, 3]. In this case, the integral THz emission intensity sharply rises when the applied electric field exceeds the impurity breakdown threshold corresponding to an increase in lateral conductivity by several orders of magnitude, as reported in [3]. The experimentally observed spectra of the acceptor-related terahertz emission demonstrate both optical transitions of hot holes to acceptor states and intracenter optical transitions between excited and ground states of an acceptor, as it was shown in [2].

The binding energy of a ground acceptor state in QWs can exceed the energy of an optical phonon, whereas the binding energy of an excited state is usually smaller. As a result, the intensity of the non-radiative capture of non-equilibrium holes to a ground acceptor state will be dramatically reduced, whereas the efficient occupation of excited acceptor states can be reached by the process of hot holes scattering from the lowest subband to the excited acceptor state with the emission of an optical phonon. This situation will facilitate hole optical transitions from the excited levels to the ground one. Therefore, the purpose of this research is to calculate the probability of non-equilibrium hole capture to the excited acceptor level with simultaneous optical phonon emission.
2. Results

2.1. The wavefunctions of excited acceptor states
In this work, we use the two-dimensional hydrogen-like model to describe the impurity state wavefunctions in QW. One can consider these functions $\xi(\vec{r})$ as a series expansion in the Bloch waves of the lowest valence subband $u_k(\vec{r})$:

$$\xi(\vec{r}) = \sum_k C(k) u_k(\vec{r}) \exp(ik\vec{r}),$$

with the serial coefficients given by the Fourier transform of the envelope wavefunction for impurity states $\psi(\vec{r})$ in $\vec{r}$-space:

$$C(k) = \frac{1}{\sqrt{S}} \int \psi(\vec{r}) \exp(-i\vec{k}\vec{r}) d^2\vec{r},$$

where $\vec{k} = \{k_x, k_y\}$ is the two-dimensional wave vector corresponding to the in-plane motion of holes, $\vec{r} = \{x, y\}$ is the two-dimensional radius vector, and $S$ is the normalizing area. In the framework of the model we use, these envelope wavefunctions for the first excited states can be expressed as $p$-like states of a two-dimensional hydrogen atom with a principal quantum number $n = 1$ and magnetic quantum numbers $m = 0, \pm 1$, and have the form [4]:

$$\psi_0(\vec{r}) = \frac{1}{\sqrt{2\pi a_0}} \frac{4}{3a_0} \left( 1 - \frac{4r}{3a_0} \right) e^{-2r/3a_0},$$

$$\psi_{21}(\vec{r}) = \frac{1}{\sqrt{2\pi}} e^{i\phi} \frac{16}{a_0 \sqrt{6}} \frac{r}{a_0} e^{-2r/3a_0},$$

where $a_0$ is the Bohr radius of a hydrogen-like impurity, and $\phi$ is the polar angle.

Thus, the serial expansion coefficients can be calculated using the Fourier transform of the excited states of the wave functions for a two-dimensional hydrogen-like impurity. After some transformations and analytical integration over $r$, we obtained these coefficients for excited acceptor states in the form:

$$C_0(\vec{k}) = \frac{1}{\sqrt{S}} \frac{1}{\sqrt{2\pi}} \frac{4a_0}{3\sqrt{3}} \int A(\phi) - 8 A'(\phi) d\phi,$$

$$C_{21}(\vec{k}) = \frac{1}{\sqrt{S}} \frac{1}{\sqrt{2\pi}} \frac{32a_0}{9\sqrt{6}} \int e^{i\phi} A(\phi) d\phi,$$

where $A(\phi) = 2/3 + ik_x a_0 \cos \phi + ik_y a_0 \sin \phi$, which cannot be further analytically simplified. The envelope wavefunctions of a two-dimensional hydrogen-like impurity and their Fourier transforms are plotted in figure 1.

2.2. The probability of scattering of non-equilibrium holes to excited acceptor states
The scheme of the intraband scattering processes with emission of optical phonons is shown in figure 2. The process marked with the arrow $a$ is a pure intraband transition with both initial $k_i$ and final $k_f$ states in the first valence subband. The two-dimensional matrix element for these intraband transitions $M_{2D}$ is calculated by P.J. Price [5]. The process marked with the arrow $b$ is the transition of interest, when the initial state is in the valence band, and the final state is the excited acceptor level.

Since we expanded the final state in the Bloch wave series according to (2.1.1), it is natural to write the squared matrix element for the transition $b$ as a product of the squared pure intraband matrix element $|M_{2D}|^2$ and the squared expansion coefficient $|C|^2$: 


Figure 1. Radial and angular parts of the two-dimensional hydrogen atom wavefunctions (a, b) and the Fourier transforms (c, d) of the excited acceptor states, respectively. The angular parts are shown as contour plots of common $p_x$–like combination (the blue lines) and $p_y$–like combination (the red lines) of the corresponding functions with $m = \pm 1$; in other words, $(\psi_{s1} + \psi_{s2})/\sqrt{2}$ and $(\psi_{s1} - \psi_{s2})/\sqrt{-2})$. The solid and dashed lines correspond to the positive and negative levels for contour plots, respectively.

Figure 2. Scheme of the intraband transition (a) and scattering to excited acceptor states (b). Energy of an optical phonon is $h\omega_0$. 
\[ |M|_z^2 = |M_{20}|_z^2 |C_{0,z1}|^2. \]  

(2.2.1)

Taking the expression for the matrix element for pure intraband polar optical scattering with the emission of an optical phonon from [5] and assuming the number of equilibrium phonons to be negligible, we can now write the probability of scattering of a hole from the state \( k_i \) in the valence subband to the state \( k_f \), that forms the excited acceptor level with the envelope \( C(k_f) \) in the form:

\[
W_{0,z1}(\vec{k}_i,\vec{k}_f) = \frac{e^2 \omega_0}{2\pi} \left( \frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0} \right) |C_{0,z1}(\vec{k}_f)|^2 \delta(E_f - E_f - h\omega_0) \int_{-\infty}^{\infty} \frac{|I(q)|^2}{Q^2 + q^2} dq, \tag{2.2.2}
\]

where \( \epsilon_0 \) and \( \epsilon_\infty \) are the static and high-frequency dielectric constants of the QW material, respectively, \( \omega_0 \) is the optical phonon frequency, \( E_f = \frac{\hbar^2 k_i^2}{2m_{hh}} \) is the initial energy, \( E_f = -\frac{4}{9} E_0 \) is the final energy (independent of \( k_f \)), and \( E_0 \) is the Rydberg constant for a three-dimensional hydrogen-like impurity in a QW material. The values of \( q \) and \( Q = k_f - k_i \) stand for the phonon wavevector projection to the growth axis and the length of a two-dimensional phonon wavevector in a QW plane, respectively. The form-factor \(|I(q)|^2\) describes the modified momentum conservation law for scattering of two-dimensional electrons on three-dimensional phonons and can be expressed in terms of a \( z \)-dependent part of the hole envelope wavefunctions in QW [5].

In order to calculate the total probability of the hole capture to the acceptor excited state, one should perform summation of the probability (2.2.2) over all phonons and average it over the distribution function \( f \) of holes in the valence band:

\[
\tau_{0,z1}^{-1} \sim \int f(\vec{k}_i) \cdot \sum Q W_{0,z1}(\vec{k}_i,\vec{k}_f) d^2\vec{k}_f. \tag{2.2.3}
\]

After summation over all the phonons, the \( \delta \)-function in (2.2.2) allows one to integrate (2.2.3) over \( k_i \) since the argument of the \( \delta \)-function is independent of \( k_f \). As a result, the total probability of the hole capture becomes proportional to the amount of holes involved in scattering due to the energy conservation:

\[
\tau_{0,z1}^{-1} \sim f(k_0), \quad k_0 = \sqrt{2m_{hh}(E_f + h\omega_0)}/\hbar. \tag{2.2.4}
\]

The proportionality coefficient includes the integration over angles and was calculated numerically.

2.3. **Time of the hole capture to excited acceptor states**

Let us now discuss the conditions of the experiment in [2,3]. One can estimate the non-equilibrium hole concentration \( p \) in the valence band to be equal to the doping level \( N_A \) since there is a full ionization of acceptors under conditions of impurity breakdown in a lateral electric field. This concentration can be expressed in terms of the distribution function \( f(E) \) and the 2D density of states \( g_{2D}(E) \):

\[
p = \int_0^\infty g_{2D}(E) f(E) dE. \tag{2.3.1}
\]

The non-equilibrium distribution function \( f(E) \) can be approximated in the concept of hot carriers for a relatively high carrier density. Under this assumption, we can write:

\[
f(E) = \left[ \exp \left( \frac{E - \mu}{k_B T_h} \right) + 1 \right]^{-1}, \tag{2.3.2}
\]

where \( T_h \) is the hot hole temperature that describes the average hole energy, \( k_B \) is the Boltzmann constant, and \( \mu \) is the quasi-Fermi-level that can be calculated from (2.3.1).
The dependences of the calculated reciprocal capture time on the hot hole temperature are shown in figure 3. At low temperatures, the contribution of optical phonon scattering is negligible due to an exponentially small amount of holes in the valence band that have enough energy to emit optical phonons. However, at high temperatures, the optical phonon contribution is significant and the probability of hole capture to an acceptor state drastically increases. For comparison, the red dotted line shows the typical high limit value for the cascade capture probability [6-8] dominating only at low temperatures.

![Figure 3](image)

**Figure 3.** Dependences of the inversed capture time on the hot hole temperature for GaAs:Be QWs with $N_A = 3.2 \times 10^{11} \text{cm}^{-2}$. QW width is equal to 3.8 nm.

Thus, the optical phonon contribution is significant for an increase in the intensity of terahertz emission related to intracenter hole transitions.

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