

## Electron-phonon scattering engineering

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We present the calculations which show that independent quantization of electrons and phonons allows the intra- and inter-subband electron-phonon scattering rate in two-dimensional structures to be changed. It is considered how the design of multi-heterostructure quantum well (QW) changes the electron mobility and population of subbands in the QW. It was shown, that the insertion of the phonon wall (a few AlAs monolayers) into an AlAs/GaAs/AlAs double heterostructure allows the electron mobility in the QW to be enhanced and electron intersubband population to be inverted.

### Introduction

In pure GaAs electron scattering by optical phonons is a dominating scattering mechanism. The electron-phonon scattering limits a value of electron mobility and determines the intersubband population of optically excited (or injected) electrons. Recently, an approach to changing the electron-optical phonon scattering rate in two-dimensional (2D) structure was proposed [1,2]. According to this approach an insertion of a phonon wall (*Ph*-wall) (a few AlAs monolayers) into an AlAs/GaAs/AlAs QW is a good tool for changing the electron-phonon scattering rate [3]. In this paper we consider an enhancement of electron mobility by inserting a *Ph*-wall into a rectangular QW and the possibilities to invert the intersubband population of optically excited electrons in the QW with a *Ph*-wall. The great increase of the electron-optical phonon scattering rate in a MODFET channel by inserting a *Ph*-wall is also considered.

### 1. Electron mobility enhancement in GaAs QW with an inserted AlAs *Ph*-wall

The division of a QW by a *Ph*-wall changes the frequencies of phonon modes, the electron-phonon coupling coefficient, and the shape of confined electron and phonon wavefunctions. As a result, the electron-optical phonon scattering rate as well as electron mobility is changed significantly [1,3].

We perform the electron-optical phonon scattering rate calculations in an AlAs/GaAs/AlAs QW with a GaAs *Ph*-wall inserted at a center of the QW (fig. 1).

The electron-phonon scattering rate is treated within the dielectric continuum approach. Considering a one-phonon process being only, considered the intrasubband (1 → 1) scattering rate of an electron with the initial wavevector  $\mathbf{k}$  by  $n$ -th mode phonon emission or absorption in the heterostructure quantized in the  $\mathbf{z}$ -direction is given by [3–5]:

$$W_{11n}(\mathbf{k}) = \frac{e^2 m}{\pi \hbar^3} \int_0^{2\pi} C_n \left( N_{qn} + \frac{1}{2} \pm \frac{1}{2} \right) \frac{|G_n|^2}{2q_n^2} d\Theta, \quad (1)$$

where  $e$  and  $m$  are the electron charge and effective mass,  $\hbar$  is Plank's constant  $N_{qn}$  is the number of  $n$ -th mode phonons, sign "+" stands for emission and "–" for absorption,

$$C_n = \left( \frac{\partial \varepsilon_n}{\partial \omega} \right)^{-1} \quad (2)$$

is the electron-phonon coupling coefficient,

$$G_n = \int_L \varphi_e^* \varphi_e \varphi_{qn} dz, \quad (3)$$

$L$  is the width of the electron QW,  $\mathbf{q}_n = \mathbf{q}_{\parallel} + \mathbf{q}_z$  is the emitted or absorbed phonon wavevector, in the plane of the heterostructure

$$q_{\parallel} = \sqrt{k^2 + k_0^2 - 2kk_0 \cos \Theta}, \quad (4)$$

$k_0 = \sqrt{k^2 - k_n^2}$ ,  $k_n = \sqrt{\frac{2m}{\hbar^2} \hbar \omega_n}$  and  $\hbar \omega_n$  is the energy of  $n$ -th mode phonon. The  $z$ -components of the electron and phonon wavefunctions  $\varphi_e$  and  $\varphi_{qn}$ , and the dielectric function  $\varepsilon_n$  are determined by the structure of a heterosystem.

The total scattering rate  $W_{11}$  is considered as a sum of the scattering rates of each  $n$ -phonon mode

$$W_{11} = \sum_n W_{11n}. \quad (5)$$

We use the slab model for confined phonon modes, thus the  $z$ -component of confined phonon potential wavefunction in the phonon well for  $z \geq 0$  is written as:

$$\varphi_q = \sqrt{\frac{2}{d_w}} \sin \left( q_z \left[ z - \frac{d}{2} \right] \right),$$

$$q_z = n \frac{2\pi}{(L-d)}, \quad n = 1, 2, \dots \quad (6)$$

where  $d_w = \frac{L-d}{2}$  is the confined phonon QW width,  $d$  is the AlAs *Ph*-wall thickness (fig. 1). The interface (IF) phonon wavefunctions in the double heterostructure with the AlAs *Ph*-wall centered at  $z = 0$  can be written for

$z \geq 0$  as:

$$\begin{aligned} \varphi_{q1} &= B \frac{\cosh(q_{\parallel} z)}{\cosh(q_{\parallel} d/2)} & z < d/2, \\ \varphi_{q21} &= B \cdot e^{-q_{\parallel}(z-d/2)} & d/2 < z < L/2, \\ \varphi_{q23} &= B \cdot e^{+q_{\parallel}(z-L/2)} & d/2 < z < L/2, \\ \varphi_{q3} &= B \cdot e^{-q_{\parallel}(z-L/2)} & z < L/2, \end{aligned} \quad (7)$$

where  $B$  is the normalization coefficient.

We have assumed that in the area  $d/2 < z < L/2$  the IF phonon wavefunctions consist of two independent branches  $\varphi_{21}$  and  $\varphi_{23}$  which have different phonon frequencies and do not interact with each other (fig. 1).

On this assumption the dielectric function  $\varepsilon$  determined from the border conditions for the wavefunction and their derivatives is different for the  $\varphi_{21}$  and  $\varphi_{23}$  branches of IF phonons:

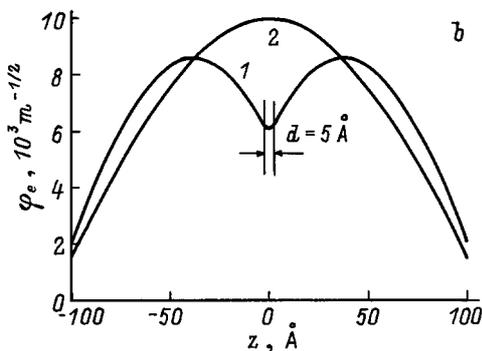
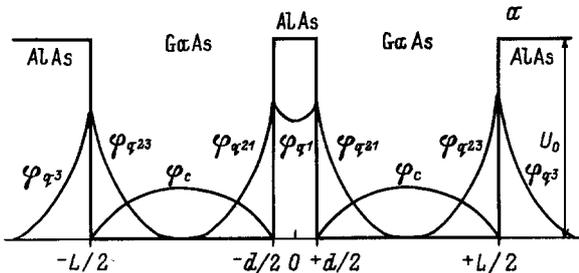
$$\varepsilon_{21} \equiv \varepsilon_1 \tanh(q_{\parallel} d/2) + \varepsilon_2 = 0, \quad \varphi_{q21} \text{ branch mode}, \quad (8)$$

$$\varepsilon_{23} \equiv \varepsilon_1 + \varepsilon_2 = 0, \quad \varphi_{q23} \text{ branch mode}, \quad (9)$$

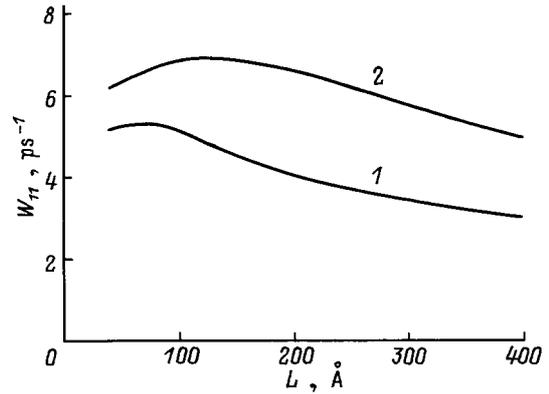
where

$$\varepsilon_{1(2)} = \varepsilon_{\infty 1(2)} \frac{\omega^2 - \omega_{L1(2)}^2}{\omega^2 - \omega_{T1(2)}^2}. \quad (10)$$

Indexes 1(2) stand for AlAs (GaAs),  $\omega_L$  and  $\omega_T$  are the longitudinal and transverse phonon frequencies, respectively,  $\varepsilon_{\infty}$  is the high frequency dielectric constant.



**Figure 1.** *a* — the double AlAs/GaAs/AlAs heterojunction QW containing the AlAs *Ph*-wall at the center of the structure. The wavefunctions of interface,  $\varphi_q$ , and confined,  $\varphi_c$ , phonon modes are shown schematically. *b* — the numerically calculated electron wavefunction in the AlAs/GaAs/AlAs QW with the AlAs *Ph*-wall of thickness  $d = 5 \text{ \AA}$  (curve 1). The electron wavefunction in the structure without the *Ph*-wall is shown for comparison (curve 2).



**Figure 2.** The rate of intrasubband electron scattering  $W_{11}$  by phonon emission in a AlAs/GaAs/AlAs QW of thickness  $L$  without (curve 2) and with (curve 1) the AlAs *Ph*-wall ( $d = 5 \text{ \AA}$ ). Electron energy  $E_e = 1.4\hbar\omega_{L2}$ ,  $T = 300 \text{ K}$ .

The frequencies of phonon modes are obtained from the dispersion equation  $\varepsilon = 0$ . Note that the frequencies and the coupling coefficients  $C_n(\omega)$  (Eq. (2)) for the  $\varphi_{q21}$  and  $\varphi_{q23}$  IF phonon modes are different.

The  $z$ -component of the lower subband electron envelope function can be approximated by the following functions (for  $z \geq 0$ ):

$$\begin{aligned} \varphi_{e1} &= A \frac{\cosh(k_1 z)}{\cosh(k_1 d/2)} & z \leq d/2, \\ \varphi_{e2} &= A \frac{\cos(k_2 z + \varphi_0)}{\cos(k_2 d/2 + \varphi_0)} & d/2 \leq z \leq L/2, \\ \varphi_{e3} &= A \frac{\cos(k_2 L/2 + \varphi_0)}{\cos(k_2 d/2 + \varphi_0)} e^{-k_1(z-L/2)} & z \geq L/2, \end{aligned} \quad (11)$$

where  $A$  is the normalization coefficient,  $k_1 = k_2 \times \sqrt{\frac{U_0}{E_1} - 1}$ ,  $k_2 = \sqrt{\frac{2m}{\hbar^2} E_1}$ , the AlAs/GaAs heterobarrier height is  $U_0 = 0.5 \text{ eV}$ ,  $E_1$  is the lower subband energy. Using boundary conditions for  $\varphi_e$  and their derivatives, the equations for the subband energy  $E_1$  and the phase  $\varphi_0$  are obtained:

$$\arctan\left(\frac{k_1}{k_2}\right) - \arctan\left(\frac{k_1}{k_2} \frac{e^{-k_1 d} - 1}{e^{-k_1 d} + 1}\right) = k_2 \frac{L - d}{2}, \quad (12)$$

$$\arctan\left(\frac{k_1}{k_2}\right) = k_2 \frac{L}{2} + \varphi_0. \quad (13)$$

It is worth mentioning that division of the GaAs QW by the AlAs barrier at its center simultaneously changes the subband energy  $E_1$  in both parts of the QW. For  $d \rightarrow 0$  and  $U_0 \rightarrow \infty$  the electron envelope function in the QW is equal to

$$\varphi_e = \sqrt{\frac{2}{L}} \cos(k_z z), \quad k_z = \pi/L.$$

In fig. 1, *b* the numerically calculated electron wavefunctions in the GaAs QW divided by the AlAs *Ph*-wall are shown.

In fig. 2 the calculated rates of the scattering of electrons with the energy of  $1.4 \cdot \hbar\omega_{1,2}$  by emission of all optical phonon modes in the AlAs/GaAs/AlAs QW without and with the inserted AlAs *Ph*-wall are shown. One can see that the insertion of the *Ph*-wall decreases the total intrasubband scattering rate more than 1.5 times in a wide range of the QW widths. This decrease is greater than that obtained in the case of an idealized QW [3]. In a pure GaAs in a wide temperature range (100÷400 K) electron scattering by polar optical phonons is a dominant mechanism that determines the electron mobility. Since the ratio of the phonon scattering rates in the GaAs QW with and without the *Ph*-wall slowly depends on the scattered electron energy, we can assume that the electron mobility changes proportionally to the scattering rate change. This means that in a pure GaAs QW with the *Ph*-wall the electron mobility increases over than 1.5 times and can reach  $1.2 \text{ m}^2/\text{V s}$  at  $T = 300 \text{ K}$ .

## 2. Intersubband scattering in a QW with *Ph*-wall

In recently demonstrated intersubband lasers the confined electron-phonon scattering is used in order to achieve the population inversion. In a three subband level laser the inverted population of electrons photoexcited from the first level to the third one is achieved when the rate of the nonradiative electron transition by phonon emission out of the third level to the second one ( $W_{32}$ ) is much less than the transition rate out of the second level to the first one ( $W_{21}$ ). The inverted population takes place when

$$\Delta n = n_3 - n_2 \approx \left(1 - \frac{W_{32}}{W_{21}}\right) n_3, \quad W_{32} \ll W_{21}. \quad (14)$$

In order to maximize the population inversion one needs to minimize nonradiative transitions between the upper levels ( $W_{32}$ ) and to maximize the transition between the lower levels ( $W_{21}$ ).

Let us consider how the insertion of the *Ph*-wall in the electron QW allows us to obtain the intersubband population inversion. For simplicity we shall consider the intersubband electron transition by emission of IF phonon only. This is a reasonable approximation in the QW with a width less than  $100 \text{ \AA}$  where the electron-IF phonon scattering rate is dominating.

The intersubband scattering rate  $W_{if}$  can be approximately written in the following form:

$$W_{if} \approx W_{oif} \frac{|G_{if}|^2}{\sqrt{E_{si} - E_{sf} - \hbar\omega_0}}, \quad (15)$$

where  $E_{si}$  and  $E_{sf}$  are the initial and final subband energies,  $\hbar\omega_0$  is the IF optical phonon energy and  $G_{if}$  is the overlap integral (3). The electron kinetic energy in initial state is assumed to be equal to zero.

The intersubband transition rate is sensitive to the design of a heterostructure due to the dependence of electron and phonon wavefunction overlap integrals and the subband energies on heterostructure parameters.

We shall consider the electron population on the first three subband levels. First of all we shall consider how the design of the electron and phonon wavefunction overlap integrals allows us to obtain population inversion. In a single QW the electron wavefunctions are symmetric on the first and third levels and asymmetric on the second level. Because of that the rate of the  $E_2 \rightarrow E_1$  transition by emission of symmetric IF phonons is very low.

In order to obtain the inversion population, one needs to maximize the  $E_2 \rightarrow E_1$  transition. The insertion of the *Ph*-wall into the electron QW splits the first subband level into two sublevels. Note that electron wavefunctions of these sublevels have the same symmetry, and the scattering rate between the sublevels increases. In the QW with the *Ph*-wall the split levels become the lower two levels in the three level laser model. The increase of  $W_{21}$  in this case creates the population inversion between the third level and the new second subband level.

The insertion of the *Ph*-wall into the QW changes the subband energies and, according to Eq.(15), the intersubband scattering rate. The intersubband scattering rate increases when the energy difference between the subbands decreases. The inversion population between the third and the second subband levels can arise when  $E_3 - E_2 > E_2 - E_1$ . Especially great is the increase of the intersubband scattering rate when the energy difference between the subbands is equal to the emitted phonon energy ( $W_{if} \rightarrow \infty$  at  $E_i - E_f - \hbar\omega_0 = 0$ ). The resonance phonon scattering is used in many papers in order to obtain population inversion in intersubband lasers (see for example [6]).

The insertion of the *Ph*-wall at the borders of MODFET channel (triangular QW) separately shifts up the energy levels of subbands with higher quantum numbers. Under conditions when the energy difference between the lower subband and the shifted subband (with the same wavefunction symmetry) is equal to emitted optical phonon energy, the resonance optical phonon scattering arises. As a result the electron mobility in the MODFET channel decreases significantly.

## Conclusions

The insertion of the *Ph*-wall into the QW is a good tool for the electron-phonon scattering engineering. The insertion of the AlAs *Ph*-wall into the center of rectangular GaAs QW enhances the electron mobility 1.5 times. The insertion of the *Ph*-wall at the borders of the MODFET channel decreases the electron mobility. The insertion of the *Ph*-wall into the QW changes the intersubband scattering rate due to the change of

symmetry of the subband electron wavefunctions as well as the intersubband energies. Both mechanisms can create the inverted population.

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