

RATE OF CONFINED PHONON EXCITATION IN RECTANGULAR QUANTUM WIRES

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Received 9 September 2011

Accepted 15 February 2012

Published 11 June 2012

We present a theory of phonon generation via the Cerenkov effect in rectangular quantum wires (RQWs) based on the quantum kinetic equation for phonon population operator. Analytical expressions for the rate of change of the phonon population and conditions for phonon generation are obtained. Both electrons and phonons are confined. Numerical results for a specific RQW show that the amplitude of the laser field must satisfy additional conditions that are different in comparison with those of the generation of bulk phonons.

Keywords: Phonon amplification; electron-phonon interaction; quantum wire; quantum kinetic equation.

1. Introduction

Phonon amplification by absorption of laser field energy has been widely investigated in bulk semiconductors [Troncini and Nunes, 1986; Nunes, 1984; Sakai and Nunes, 1987; Epshtein, 1971] and in low-dimensional heterostructures in which the electron systems are two-dimensional [Sakai and Nunes, 1990; Zhao, 1994; Komirenko *et al.*, 2000a, 2000b, 2001a, 2001b, 2002; Glavin *et al.*, 1999, 2002; Peng, 1994] and one-dimensional [Peng, 1999; Totland *et al.*, 1999]. These studies provide information on the excitation mechanisms of phonons, their dynamics, electron-phonon interactions and other important phenomena. The main results of these works are that if the current is due to electron motion in an electric field, phonon amplification (generation) can be achieved via the Cerenkov effect when the electron drift velocity exceeds the phase velocity of the phonons.

High-frequency phonons have been observed for a number of semiconductor materials and heterostructures: GaAs and Ge [Kutt, 1992], as well as other materials [Merlin, 1997] (see Komirenko *et al.* [2000a, 2001a, 2002] and Glavin [2002] for a recent review). In quantum semiconductor heterostructures, if the current is due

to transitions of carriers between the bound-electron states, generation of phonons can be realized if population inversion of these states occurs. Similar effects for photon generation have been demonstrated in cascade lasers [Faist, 1994]. Intense phonon waves can be exploited for various applications; these include [Komirenko *et al.*, 2000a, 2001a, 2002; Glavin, 2002; Hill *et al.*, 1997; Hu and Nori, 1999] the classical problem of sound amplification by drifting electrons, the modulation of optical signals, the modulation of electric current, phonon active control of electron transport, short-wavelength phonon induced phototransitions in indirect gap semiconductors, heat removal through stimulated phonon decay and nondestructive testing of nanostructures (phonon wavelengths can be scaled down to 10 nm).

It is important to note that both theoretical analysis and experiments [Özgür *et al.*, 2001] have shown that phonon generation by drifting electrons in bulk semiconductor is practically impossible because the rate of phonon generation cannot compete with the large rate of phonon losses. However, advanced technology of semiconductor heterostructures has opened new possibilities for applying the Cerenkov effect for phonon generation, especially for acoustic phonon generation because electron drift velocities and electron densities in low-dimensional systems are much greater than they are in bulk samples. Due to a necessarily strong coupling of electrons and phonons in the same quantum well of quantum wires, we expect phonon generation via the Cerenkov effect to be now capable of competing with phonon losses.

Phonon amplification by absorption of laser field energy can be considered phenomenologically by using the kinetic equation for the phonon population which corresponds to the transition probability per unit time [Troncini and Nunes, 1986; Nunes, 1984; Sakai and Nunes, 1987; Zhao, 1994; Peng, 1994, 1999; Totland *et al.*, 1999] or the Boltzmann equation. However, Herbst *et al.* [2003] have shown that carrier-phonon scattering processes on the quantum kinetic level are described by the dynamics of phonon assisted density matrices. Since in the Boltzmann equation, the scattering rates due to different interaction mechanisms simply add up without interference, all contributions to the quantum kinetic equation resulting from mechanisms other than carrier-phonon interactions have to be neglected. This shows that the quantum kinetic treatment includes a variety of additional phenomena related to the mutual influence of different mechanisms, besides the correct treatment of the short time- and length-scale behavior. In particular, the carrier-phonon scattering dynamic is modified by intraband and interband Fock terms, external fields, etc. Recently, one of the authors (Phong, T. C.) [Phong and Dung, 2004] studied phonon amplification in semiconductor superlattices by using the quantum kinetic equation in the case of multi-photon absorption processes.

In this paper, we study the influence of phonon confinement on phonon generation rate in rectangular quantum wires (RQWs). This is fairly different in comparison to previous results. Starting from the kinetic equation for the phonon, we calculate the rate of phonon population change and find the conditions for

phonon generation. Analytical expressions for the rate of phonon excitation and the conditions are obtained for the case of the multi-photon absorption process and a non-degenerate electron gas. The mechanism and the specific characteristics of the phonon generation are illustrated for a realistic quantum wire model.

This paper is organized as follows. In Sec. 2, we establish the quantum kinetic equation for confined phonons in RQWs under a laser field. In Sec. 3, we calculate the rate of change of the phonon population in RQWs. For definiteness, in Sec. 4, we offer numerical results for a specific model GaAs/AlAs system. Conclusions are given in Sec. 5.

2. Quantum Kinetic Equation for a Phonon in RQWs

Let us consider a quantum wire of rectangular cross section along the z axis, with finite x and y dimensions given, respectively by L_x and L_y . We assume that the walls are impenetrable; that is, the confining potential well is an infinite square well. In this case, the state and the electron energy spectra have the form [Stroscio, 1989]

$$|\ell, j, k_z\rangle \equiv |\alpha, k_z\rangle = \frac{e^{ik_z z}}{\sqrt{L_z}} \frac{2}{\sqrt{L_x L_y}} \cos\left(\frac{\pi \ell x}{L_x}\right) \cos\left(\frac{\pi j y}{L_y}\right), \quad (1)$$

$$\varepsilon_{\ell, j}(k_z) \equiv \varepsilon_{\alpha}(k_z) = \frac{\hbar^2 k_z^2}{2m_e} + \frac{\pi^2 \hbar^2}{2m_e} \left(\frac{\ell^2}{L_x^2} + \frac{j^2}{L_y^2} \right) = \frac{\hbar^2 k_z^2}{2m_e} + \varepsilon_{\alpha}, \quad (2)$$

where k_z is the electron wave vector along the wire's z axis and m_e is the electron effective mass, L_z is the length of the RQW, $-L_x/2 \leq x \leq L_x/2$ and $-L_y/2 \leq y \leq L_y/2$.

Here, we are interested in the role of phonons. With the confined optical phonon assumption, Hamiltonian of the electron-phonon system in RQWs in the presence of a laser field, $\vec{E} = \vec{E}_0 \sin \Omega t$, is written as [Kang *et al.*, 2004; Yu, 2008]

$$H(t) = \sum_{\alpha, k_z} \varepsilon_{\alpha} \left(\mathbf{k} - \frac{e}{\hbar c} \mathbf{A}(t) \right) c_{\alpha}^{\dagger}(k_z) c_{\alpha}(k_z) + \sum_{m, n, q_z} \hbar \omega_0 a_{m, n}^{\dagger}(q_z) a_{m, n}(q_z) \\ + \sum_{\alpha, \alpha'} \sum_{m, n, k_z, q_z} M_{\alpha, \alpha'}^{m, n}(q_z) c_{\alpha'}^{\dagger}(k_z + q_z) c_{\alpha}(k_z) (a_{m, n}(q_z) + a_{m, n}^{\dagger}(-q_z)) \quad (3)$$

where $c_{\alpha}^{\dagger}(k_z)$ and $c_{\alpha}(k_z)$ ($a_{m, n}^{\dagger}(q_z)$ and $a_{m, n}(q_z)$) are the creation and the annihilation operators of confined electron (phonon) for state $|\alpha, k_z\rangle$ ($|m, n, q_z\rangle$) respectively; $\mathbf{k} = (0, 0, k_z)$; k_z and q_z are the components along the z -axis of confined electron and phonon wave vector; $\mathbf{A}(t)$ is the vector potential of the external field; $M_{\alpha, \alpha'}^{m, n}(q_z) = \gamma I_{\alpha, \alpha'}^{m, n}(q_z)$, the electron-phonon interaction matrix element, depends on the scattering mechanism and is given by (within the infinite square potential confinement model) [Stroscio, 1989]

$$I_{\alpha, \alpha'}^{m, n}(q_z) = \frac{(2\pi)^2}{L_y L_y} \left| \sum_{m, n=1, 3, 5, \dots} 4P_{\alpha, \alpha'}^{m, n} \left[q_z^2 + \left(\frac{m\pi}{L_x} \right)^2 + \left(\frac{n\pi}{L_y} \right)^2 \right]^{-1/2} \right|^2, \quad (4)$$

where [Campos, 1992]

$$P_{\alpha,\alpha'}^{m,n} = \frac{4}{L_x L_y} \int_{-L_x/2}^{L_x/2} dx \int_{-L_y/2}^{L_y/2} dy \cos\left(\frac{\pi \ell x}{L_x}\right) \cos\left(\frac{\pi j y}{L_y}\right) \times \cos\left(\frac{\pi \ell' x}{L_x}\right) \cos\left(\frac{\pi j' y}{L_y}\right) \zeta_m(x) \zeta_n(y). \quad (5)$$

The function ζ_m , which is determined by the confinement mode, is defined as follows for the slab modes

$$\zeta_m(x) = \sin\left(\frac{m\pi x}{L_x} + \frac{\pi}{2}\delta_m\right), \quad (6)$$

and for the guided modes

$$\zeta_m(x) = \cos\left(\frac{m\pi x}{L_x} + \frac{\pi}{2}\delta_m\right), \quad (7)$$

and γ , the confined electron- optical phonon interaction constant, takes the form

$$\gamma = \left[\frac{2\pi e^2 \hbar \omega_0}{V} \left(\frac{1}{\chi_\infty} - \frac{1}{\chi_0} \right) \right]^{1/2} \quad (8)$$

The quantum kinetic equation for phonons (average phonon number) in RQWs is

$$i\hbar \frac{\partial}{\partial t} \langle a_{m,n}^+(q_z) a_{m,n}(q_z) \rangle_t = i\hbar \frac{\partial N_{m,n,q_z}(t)}{\partial t} = \langle [a_{m,n}^+(q_z) a_{m,n}(q_z), H(t)] \rangle_t, \quad (9)$$

where $\langle X \rangle_t$ means the usual thermodynamic average of X at moment t . Using $H(t)$ and realizing operator algebraic calculations, we have

$$\frac{\partial N_{m,n,q_z}(t)}{\partial t} = \frac{i}{\hbar} \sum_{\alpha,\alpha',k_z} [M_{\alpha,\alpha'}^{m,n}(q_z) F_{\alpha,k_z}^{\alpha',k_z+q_z}(m,n,q_z,t) - M_{\alpha,\alpha'}^{m,n}(q_z) F_{\alpha',k_z-q_z}^{\alpha,k_z}(m,n,q_z,t)^*], \quad (10)$$

where

$$F_{\alpha,\mathbf{k}}^{\alpha',\mathbf{k}'}(m,n,q_z,t) \equiv F(t) = \langle c_\alpha^+(q_z) c_{\alpha'}(k_z - q_z) a_{m,n}(q_z) \rangle_t. \quad (11)$$

Continuously, we write the quantum kinetic equation for $F(t)$ in the form (9) by utilizing above Hamiltonian, then by solving it by using the method of constant variation with the assumption of an adiabatic interaction, $F(t)|_{t \rightarrow -\infty} = 0$, we obtain the quantum kinetic equation for phonons in RQWs.

$$\frac{\partial N_{m,n,q_z}(t)}{\partial t} = \frac{1}{\hbar^2} \sum_{\alpha,\alpha',k_z} |M_{\alpha,\alpha'}^{m,n}(q_z)|^2 \sum_{s=-\infty}^{\infty} J_s^2\left(\frac{\Lambda}{\hbar\Omega}\right) \int_{-\infty}^t dt' N_{m,n,q_z}(t') \times \left\{ [f_{\alpha'}(k_z + q_z) - f_\alpha(k_z)] \exp\left[\frac{i}{\hbar}(\varepsilon_{\alpha'}(k_z + q_z) - \varepsilon_\alpha(k_z))\right] \right.$$

$$\begin{aligned}
 & -\hbar\omega_0 - s\hbar\Omega)(t - t')] + [f_\alpha(k_z) - f_{\alpha'}(k_z - q_z)] \\
 & \times \exp\left[\frac{i}{\hbar}(\varepsilon_{\alpha'}(k_z - q_z) - \varepsilon_\alpha(k_z) + \hbar\omega_0 + s\hbar\Omega)(t - t')\right] \Big\}, \quad (12)
 \end{aligned}$$

where $f_\alpha(k_z)$ is the distribution function of the electron gas, which is assumed to be in equilibrium, and $\Lambda = e\hbar q_z E_0 / (m_e \Omega)$ is the field parameter.

3. Rate of the Phonon Population Change

Using the Fourier transform technique and the assumption of an adiabatic interaction of the laser field, one obtains the kinetic equation for the phonon population of the q_z mode [Troncini and Nunes, 1986; Nunes, 1984; Sakai and Nunes, 1987]:

$$\frac{\partial N_{m,n,q_z}(t)}{\partial t} = G_{m,n,q_z} N_{m,n,q_z}(t), \quad (13)$$

where G_{m,n,q_z} is a parameter that determines the rate of change of the phonon population $N_{m,n,q_z}(t)$ in time due to the interaction with electrons and takes the following form:

$$\begin{aligned}
 G_{m,n,q_z} &= \frac{2\pi}{\hbar} \sum_{\alpha,\alpha',k_z} |M_{\alpha,\alpha'}^{m,n}(q_z)|^2 \sum_{s=-\infty}^{+\infty} J_s^2\left(\frac{\Lambda}{\hbar\Omega}\right) [f_{\alpha'}(k_z + q_z) - f_\alpha(k_z)] \\
 &\times \delta(\varepsilon_{\alpha'}(k_z + q_z) - \varepsilon_\alpha(k_z) - \hbar\omega_0 - s\hbar\Omega). \quad (14)
 \end{aligned}$$

The parameter G_{m,n,q_z} has significant meaning; that is, if $G_{m,n,q_z} > 0$, the phonon population grows with time (phonon amplification) whereas for $G_{m,n,q_z} < 0$, the phonons are damped. In the strong-field limit, $\Lambda \gg \hbar\Omega$, the sum over s in Eq. (14) may then be written approximately as [Troncini and Nunes, 1986; Nunes, 1984; Sakai and Nunes, 1987]

$$\sum_{s=-\infty}^{+\infty} J_s^2\left(\frac{\Lambda}{\hbar\Omega}\right) \delta(\varepsilon - s\hbar\Omega) = \frac{1}{2}[\delta(\varepsilon - \Lambda) + \delta(\varepsilon + \Lambda)], \quad (15)$$

with

$$\varepsilon = \varepsilon_{\alpha'}(k_z + q_z) - \varepsilon_\alpha(k_z) - \hbar\omega_0.$$

The first Delta function corresponds to the emission and the second to the absorption of $(\Lambda/\hbar\Omega)$ photons. In other words, in the strong-field limit, only multiphoton processes are dominant and the electron-phonon interaction takes place with the emission and the absorption of $(\Lambda/\hbar\Omega) \gg 1$ photons. Substituting Eq. (15) into Eq. (14), the rate of phonon population change becomes $G_{m,n,q_z} = G_{m,n,q_z}^{(+)} + G_{m,n,q_z}^{(-)}$, where

$$\begin{aligned}
 G_{m,n,q_z}^{(\pm)} &= \frac{\pi}{\hbar} \sum_{\alpha,\alpha',k_z} |M_{\alpha,\alpha'}^{m,n}(q_z)|^2 [f_{\alpha'}(k_z + q_z) - f_\alpha(k_z)] \\
 &\times \delta[\varepsilon_{\alpha'}(k_z + q_z) - \varepsilon_\alpha(k_z) - \hbar\omega_0 \pm \Lambda]. \quad (16)
 \end{aligned}$$

Transforming the sum over k_z to an integral in k_z space and assuming that the electron gas is non-degenerate, we substitute expressions for the energy spectra and the Fermi-Dirac distribution function, $f_\alpha(k_z) = \exp[\beta(\varepsilon_F - \varepsilon_\alpha(k_z))]$ and by carrying out some calculations, we get the expressions for $G_{m,n,q_z}^{(\pm)}$ as follows

$$G_{m,n,q_z}^{(\pm)} = \frac{Lm_e}{2\hbar^3q_z} \sum_{\alpha,\alpha'} |M_{\alpha,\alpha'}^{m,n}(q_z)|^2 \times \left\{ \exp \left[\beta \left(\varepsilon_F - \varepsilon_{\alpha'} - \frac{\hbar^2}{m_e} \left(\frac{m_e}{\hbar^2q_z} (\Delta\varepsilon + \hbar\omega_0 \mp \Lambda) - q_z \right)^2 \right) \right] - \exp \left[\beta \left(\varepsilon_F - \varepsilon_\alpha - \frac{m_e}{2\hbar^2q_z^2} (\Delta\varepsilon + \hbar\omega_0 \mp \Lambda)^2 \right) \right] \right\}, \quad (17)$$

here, ε_F is the Fermi energy, $\beta = 1/(k_B T)$, k_B is the Boltzmann constant, T is the temperature of the system and

$$\Delta\varepsilon = \varepsilon_{\alpha'} - \varepsilon_\alpha - \frac{\hbar^2q_z^2}{2m_e}.$$

From Eq. (17), we can derive the conditions for the phonon generation. It can be seen that only the multi-photon absorption process ($\Lambda/(\hbar\Omega) \gg 1$) corresponding to the signs (+) in the superscript of G_{m,n,q_z} and the signs (-) in front of Λ satisfy the condition $G_{m,n,q_z}^{(+)} > 0$ for phonon generation. In this case, we obtain the condition that laser field must satisfy

$$\Lambda = \frac{e\hbar q_z E_0}{m_e \Omega} > \hbar\omega_0. \quad (18)$$

The condition in Eq. (18) simply means that for a particular phonon wave vector, the necessary condition for the onset of the phonon instability is just the Cerenkov condition $q_z v_0 > \omega_0$, where $v_0 = eE_0/(m_e \Omega)$ and $v_{ph} = \omega_0/q_z$ is the phonon-phase velocity. The above result is formally analogous to the one for the electron-phonon system in the presence of a dc electric field. The difference lies in the fact that in the latter case, \mathbf{v}_0 is replaced by the drift velocity $\mathbf{v}_d = eE_0/(m_e \Omega)$ imposed by the static field [Troncini and Nunes, 1986; Nunes, 1984; Sakai and Nunes, 1987; Peng, 1994].

4. Numerical Results and Discussion

For a deeper insight of the problem of phonon excitation, we present detailed numerical calculations of the rate of the phonon population change, G_{m,n,q_z} for a model of RQW in this section. For the numerical evaluation, we consider the model of a RQW of GaAs/AlAs with the following parameters [Yu *et al.*, 2006; Wang and Lei, 1994]: $\chi_\infty = 10.89$, $\chi_0 = 13.18$, $m = 0.067m_0$ (m_0 being the mass of free electron), $\hbar\omega_0 = 36.6$ meV, $L_y = 100$ nm, $L_z = 500$ nm, $\varepsilon_F = 0.5 \times 10^{-18}$ J, $E_0 = 5 \times 10^6$ Vm $^{-1}$.

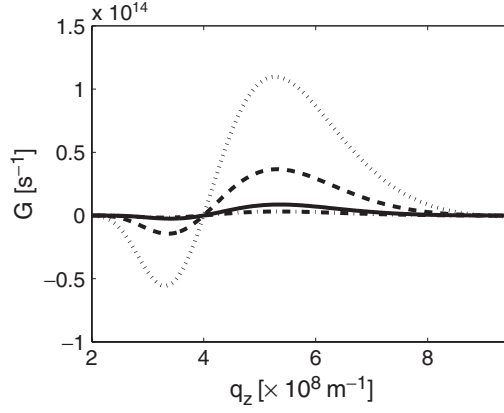


Fig. 1. The dependence of the phonon generation rate on the wave number for two cases: confined LO phonon (at different lattice temperature: the solid, the dashed, and the dotted lines correspond to 200 K, 230 K and 260 K respectively) and bulk LO phonon (dashed-dotted line at 260 K). Here, the laser field frequency is 4.0×10^{13} Hz, the length L_x of RQW is 100 nm.

The transition included in the numerical results is $\ell = 2$, $\ell' = 1$, $j = j' = 1$, $m = n = 1$.

Figure 1 shows the dependence of G_{m,n,q_z} on the phonon's wave number q_z at different values of the temperature. It can be seen that the rate of phonon population change has both the positive (amplification) and negative (absorption) values for confined phonons. For each curve, the phonon generation rate, G_{m,n,q_z} , has the minimum negative value as the wave number, q_z , increased. It changes the sign at $q_z \approx 4 \times 10^8 \text{ m}^{-1}$, then reaches the maximum and decreases exponentially at high q_z . This means that only confined phonons with wave number larger than $4 \times 10^8 \text{ m}^{-1}$ can be created and phonons with wave number less than that are almost absorbed. In other words, the phonon amplification occurs at the same value of wave number for different temperatures. This behavior was also observed by Komirenko *et al.* [2000a, 2001a, 2002] and Glavin [2002]. The most interesting thing in the present work is that the value of q_z at which G_{m,n,q_z} reaches maximum or minimum does not depend on the temperature. Moreover, the higher the temperature, the greater the rate of phonon amplification and their absorption. Figure also shows that if the phonon's wave number is greater than $9 \times 10^8 \text{ m}^{-1}$, the influence of the phonon confinement has nearly disappeared, implying that the external field has no impact on the phonon excitation.

The dependence of the rate of the phonon population change on the length L_x of RQW is shown in Fig. 2 for different values of laser field frequency. This dependence can be described similarly as in Fig. 1. We can see that the rate of the phonon population change for confined phonons possesses both positive and negative value. At the given parameters, the increase in the laser field frequency shifts the maximum of G_{m,n,q_z} to smaller wave numbers and the minimum to the

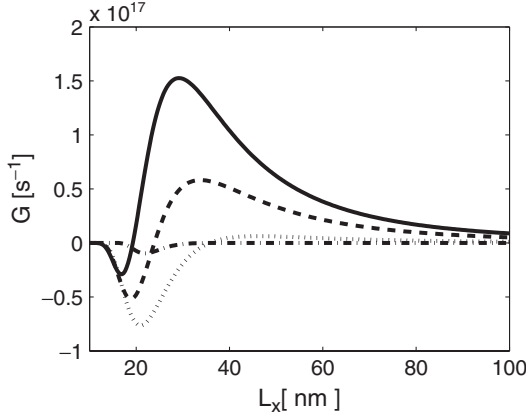


Fig. 2. The dependence of the LO phonon generation rate on the length L_x of RQW for two cases: confined LO phonon at different values of the laser field frequency — the solid, the dashed, and the dotted lines correspond to $\Omega = 3.5 \times 10^{13}$ Hz, 4×10^{13} Hz, and 4.5×10^{13} Hz respectively and bulk LO phonon (dashed-dotted line) at $\Omega = 4 \times 10^{13}$ Hz. Here, the wavenumber q_z is $4 \times 10^8 \text{ m}^{-1}$, $T = 260$ K.

larger wave numbers. Furthermore, the values of confined phonon generation or absorption are much greater than they are in the case of bulk phonons.

5. Conclusions

In conclusion, we have analytically investigated the possibility of phonon generation by absorption of laser-field energy in a rectangular quantum wire in the case of a multiphoton absorption process and a non-degenerate electron gas. Starting from the confined phonon assumption and using the quantum kinetic equation for phonons, we have obtained expressions for the rate of change of the phonon population in the cases of confined optical phonons.

The expressions are numerically calculated and plotted for a specific RQW to show the mechanism of phonon generation. The obtained results show that the impact of the phonon confinement is considerable for optical phonon with the sufficient small wavenumber and the length of RQW. This impact is insignificant for phonons with large wavenumber as well as the length of RQW.

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