Computational Materials Science 49 (2010) S260–S262

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

# Calculation of the nonlinear absorption coefficient of a strong electromagnetic wave by confined electrons in quantum wires

Le Thi Thu Phuong [a], Huynh Vinh Phuc [b], Tran Cong Phong [a,*]

[a] Hue University's College of Education, 32 Le Loi Str., Hue City, Viet Nam
[b] Dong Thap University of Education, 783 Pham Huu Lau Str., Dong Thap, Viet Nam

ARTICLE INFO

*Article history:*
Received 4 October 2009
Received in revised form 1 March 2010
Accepted 4 March 2010
Available online 9 April 2010

*Keywords:*
Cylindrical quantum wires
Nonlinear absorption coefficient
Quantum kinetic equation

ABSTRACT

General analytic expressions for the absorption coefficient (ACF) of a strong electromagnetic wave (SEM) caused by confined electrons in cylindrical quantum wires (CQW) are obtained by using the quantum kinetic equation for electrons in the case of electron–optical phonon scattering. Second-order multiphoton process is included into the result. The dependence of ACF on the amplitude $E_0$ and the energy $\hbar\Omega$ of a SEM, the temperature $T$ of the system, and radius $R$ of CQW for a specific CQW GaAs/AlAs is achieved due to numerical method. The computational results show that the dependence of ACF on $\hbar\Omega$ and $R$ can be applied to optically detect the electric subbands in a CQW.



## 1. Introduction

In low-dimensional structures, the energy levels of electrons become discrete and are different from other dimensionalities [1]. In certain conditions, the decrease in dimensionality of system for semiconductors can lead to a dramatically enhancement of nonlinearities [2]. So the nonlinear optical properties of semiconductor quantum wells, quantum wires, and quantum dots have attracted much attention in the past few years.

Linear and nonlinear optical absorption in low-dimensional structures have been extensively studied experimentally and theoretically in the past [3,4]. So far, however, almost all classical and quantum mechanical treatments on this problem were based on the perturbation expansion of the interaction between electrons and phonons, mostly with only the single-photon process included, and thus limited to the case of weak radiation fields. In the present work, we study the nonlinear optical absorption of a SEM by confined electrons in CQW. Present work is fairly different in comparison to the previous results [5] because two-photon absorption process is included and we show that present results can be applied to optically detect the electric subbands in a CQW.

The paper is organized as follows. In the next section we outline a QKE for electron confined in a CQW and the general analytical expression for ACF in the case of electron–optical phonon scattering mechanism. The numerical results are presented for GaAs/AlAs cylindrical quantum wires in Section 4. Finally, brief conclusions are given in Section 5.

## 2. Model of a CQW and quantum transport equation for electrons

We consider a CQW of polar semiconductors consisting of GaAs embedded in AlAs. The one-particle total wave function in cylindrical coordinates $(r,\phi,z)$ takes the form

$$\psi_{n,\ell,k_z}(r,\phi,z)=\frac{1}{\sqrt{V_0}}e^{in\phi}e^{ik_z z}\psi_{n,\ell}(r), \tag{1}$$

where $V_0=\pi R^2 L_z$ is the volume of the wire, $n=0,\pm1,\pm2,\ldots$ is the azimuthal quantum number, $\ell=1,2,3,\ldots$ is the radial quantum number; $\vec{k}=(0,0,k_z)$ is the electron wave vector, and $\psi_{n,\ell}(r)$ is the radial wave function which has the form

$$\psi_{n,\ell}(x)=\frac{1}{J_{n+1}(B_{n,\ell})}J_n(B_{n,\ell}x),\quad x=r/R, \tag{2}$$

and energy levels of the system can be worked out by $E_{n,\ell}(k)=E(k_z)+E_{n,\ell}$, where $E(k_z)=\hbar k_z^2/(2m)$ is the energy in the axial direction, $E_{n,\ell}(0)=\frac{\hbar^2}{2m}\left(\frac{B_{n,\ell}}{R}\right)^2$, where $B_{n,\ell}$ is the $\ell$th zero of the $n$th order Bessel function (for example, $B_{0,1}=2.405$ and $B_{1,1}=3.832$) and $m$ is the electronic effective mass.

The Hamiltonian of the electron–optical phonon system in the presence of a SEM can be written as $H=H_0+U$, in which [6]:

* Corresponding author.
*E-mail address:* congphong2000@yahoo.com (T.C. Phong).

0927-0256/$ - see front matter © 2010 Elsevier B.V. All rights reserved.
doi:10.1016/j.commatsci.2010.03.004

$$H_0 = \sum_{n,\ell,k_z} \varepsilon_{n,\ell}\left(\vec{k}_z - \frac{e}{\hbar c}\vec{A}(t)\right) a^+_{n,\ell,k_z} a_{n,\ell,k_z} + \sum_{\vec{q}} \hbar\omega_{\vec{q}} b^+_{\vec{q}} b_{\vec{q}}, \tag{3}$$

$$U = \sum_{n,n',\ell,\ell'} \sum_{k_z,\vec{q}} C_{\vec{q}} M_{n,\ell,n',\ell'}(q_\perp) a^+_{n',\ell',\vec{k}_z+\vec{q}_z} a_{n,\ell,\vec{k}_z}(b_{\vec{q}} + b^+_{-\vec{q}}), \tag{4}$$

where $(n,\ell,k_z)$ and $(n',\ell',k_z+q_z)$ are electron states before and after scattering, $a^+_{n,\ell,k_z}$ and $a_{n,\ell,k_z}$ ($b^+_{\vec{q}}$ and $b_{\vec{q}}$) denote the creation and annihilation operators of electron (phonon) respectively, $\vec{q} = (q_\perp, q_z)$ being the phonon wave vector, $\vec{A}(t)$ is the vector potential of the SEM, $\vec{A}(t) = \frac{e}{\Omega}\vec{E}_0 \sin\Omega t$; $e$ is the electron charge; $C_{\vec{q}}$ is the electron–phonon interaction factor and depends on the scattering mechanism, it means that for electron–optical phonon interaction with $\omega_q = \omega_0$, $C_{\vec{q}}$ is [7]: $C_{\vec{q}} = \frac{ie}{q}\left(\frac{\hbar\omega_0}{2\epsilon_0 V_0}\left(\frac{1}{\chi_\infty} - \frac{1}{\chi_0}\right)\right)^{1/2}$, where $\epsilon_0$ is the electronic constant; $\chi_0$ and $\chi_\infty$ are the static and the high-frequency dielectric constant, respectively; and the matrix element $M_{n,\ell,n',\ell'}(q_\perp)$ characterizes the confinement of electrons in the CQW and takes the form [8]

$$M_{n,\ell,n',\ell'}(y) = \int_0^1 x J_{|n-n'|}(yx)\psi^*_{n',\ell'}(x)\psi_{n,\ell}(x)dx, \tag{5}$$

where $y = q_\perp R$.

In order to establish a QKE for electrons in CQW, we use the general quantum equation for the particle number operator (or electron distribution function) $f_{n,\ell,k_z} = \left\langle a^+_{n,\ell,k_z} a_{n,\ell,k_z}\right\rangle_t$:

$$i\hbar\frac{\partial f_{n,\ell,k_z}(t)}{\partial t} = \left\langle\left[a^+_{n,\ell,k_z} a_{n,\ell,k_z}, H\right]\right\rangle_t, \tag{6}$$

where $\langle\psi\rangle_t$ denotes a statistical average value at the moment $t$, $\langle\psi\rangle_t = Tr(\widehat{W}\widehat{\psi})$ ($\widehat{W}$ is the density matrix operator).

Starting from the Hamiltonian $H$ and using the commutation relations of creation and annihilation operators, we obtain a QKE for electrons in a CQW. Solving the equation as in Ref. [9], we get the expression for the electron distribution function.

## 3. General analytic expression of ACF in a CQW

Because the motion of electrons is confined in $(x—y)$ plane, we consider only the current density vector along the $z$-direction. As in Ref. [9], using the $z$-component of the current density in a CQW

$$j_z(t) = \frac{e\hbar}{m}\sum_{n,\ell,k_z}\left(\vec{k}_z - \frac{e}{\hbar c}\vec{A}(t)\right) f_{n,\ell,k_z}(t), \tag{7}$$

the absorption coefficient takes the form

$$\alpha = \frac{8\pi}{c\sqrt{\chi_\infty}E_0^2}\langle j_z(t)E_0\sin\Omega t\rangle_t. \tag{8}$$

Finally, calculating the summations with respect to $k_z$ and then the summations with respect to $\vec{q}$, we obtain a general analytical result

$$\begin{aligned}\alpha = {} & \frac{e^4 k_B T}{8\pi c\sqrt{\chi_\infty}\Omega^3 m\hbar^2\varepsilon_0 V_0}\left(\frac{1}{\chi_\infty} - \frac{1}{\chi_0}\right)\sum_{n,\ell,n',\ell'}\exp\left(\frac{1}{k_B T}\left(\varepsilon_F - \frac{\hbar^2 B^2_{n,\ell}}{2mR^2}\right)\right)\\ & \times H_{n,\ell,n',\ell'}\left\{\sum_{i=1}^{2}\exp\left(\frac{C_i}{2k_B T}\right)K_0\left(\frac{C_i}{2k_B T}\right)\right.\\ & + \sum_{i=3}^{4}\exp\left(\frac{-C_i}{2k_B T}\right)K_0\left(\frac{C_i}{2k_B T}\right)\\ & + \frac{1}{2}\left(\frac{eE_0}{2m\Omega^2}\right)^2\left[\sum_{i=1}^{2}\left(\frac{D_i}{2k_B T}\right)\exp\left(\frac{2mD_i}{\hbar^2}\right)K_1\left(\frac{D_i}{2k_B T}\right)\right.\\ & \left.\left. + \sum_{i=3}^{4}\left(\frac{2mD_i}{\hbar^2}\right)\exp\left(\frac{-D_i}{2k_B T}\right)K_1\left(\frac{D_i}{2k_B T}\right)\right]\right\},\end{aligned} \tag{9}$$

$$H_{n,\ell,n',\ell'} = \int_0^\infty q_\perp |M_{n,\ell,n',\ell'}(q_\perp)|^2 dq_\perp, \tag{10}$$

$$C_i = -\frac{\hbar^2 B^2_{n',\ell'}}{2mR^2} + \frac{\hbar^2 B^2_{n,\ell}}{2mR^2} \mp \hbar\omega_0 - \hbar\Omega, \quad \text{for } i = 1,2, \tag{11}$$

$$C_i = \frac{\hbar^2 B^2_{n',\ell'}}{2mR^2} - \frac{\hbar^2 B^2_{n,\ell}}{2mR^2} \mp \hbar\omega_0 - \hbar\Omega, \quad \text{for } i = 3,4, \tag{12}$$

$$D_i = -\frac{\hbar^2 B^2_{n',\ell'}}{2mR^2} + \frac{\hbar^2 B^2_{n,\ell}}{2mR^2} \mp \hbar\omega_0 - 2\hbar\Omega, \quad \text{for } i = 1,2, \tag{13}$$

$$D_i = \frac{\hbar^2 B^2_{n',\ell'}}{2mR^2} - \frac{\hbar^2 B^2_{n,\ell}}{2mR^2} \mp \hbar\omega_0 - 2\hbar\Omega, \quad \text{for} \quad i = 3,4. \tag{14}$$

The present result yields a more specific and significant interpretation of the electronic processes for emission and absorption of phonons and photons. The third and fourth terms are the contributions of the two-photon process. These analytical results appear very involved. However, physical conclusions can be drawn from graphical representations and numerical results, obtained from adequate computational methods.

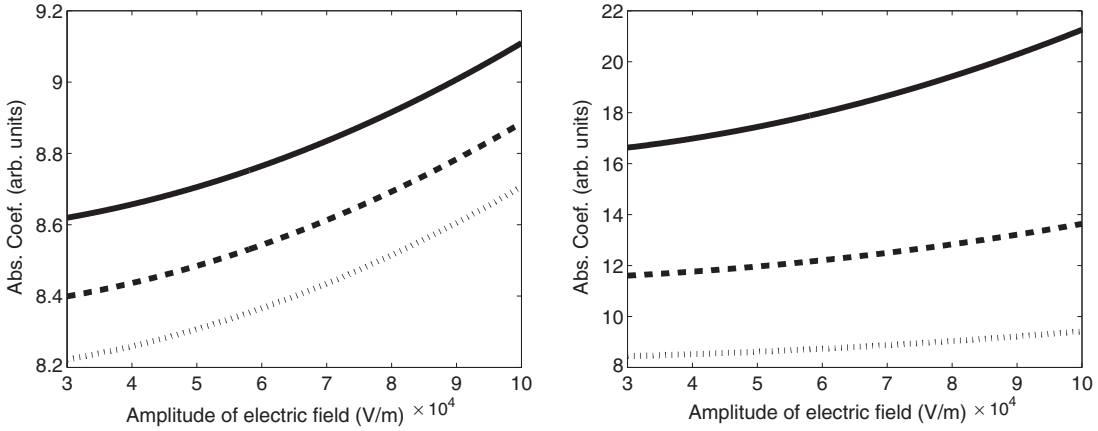


**Fig. 1.** Absorption coefficient (arb. units) as a function of the amplitude $E_0$ at (a) on the left: temperature of 240 K (solid line), 250 K (dashed line), and 260 K (dotted line), where the laser field energy is $\hbar\Omega = 29.5$ meV, and (b) on the right: photon energy of 29.5 meV (solid line), 30.2 meV (dashed line), and 30.8 meV (dotted line), where temperature is $T = 250$ K.

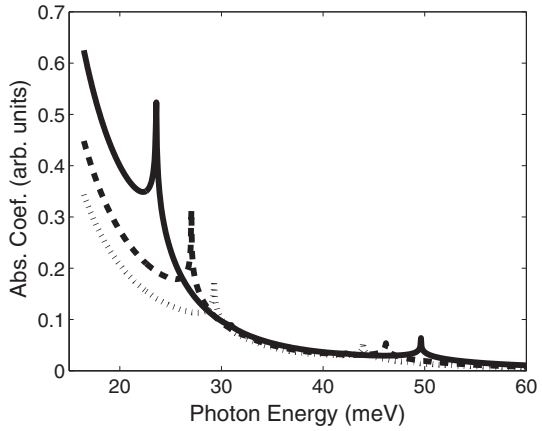


**Fig. 2.** Absorption coefficient (arb. units) as a function of photon energy at different values of the radius $R$: $R = 30$ nm (solid line), $R = 35$ nm (dashed line), and $R = 40$ nm (dotted line). Here, $T = 250$ K, $E_0 = 4.0 \times 10^4$ V/m.

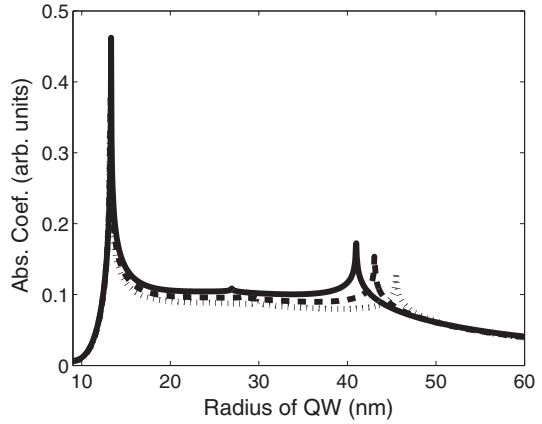


**Fig. 3.** Absorption coefficient (arb. units) as a function of radius $R$ at the different photon energy: photon energy of 29.5 meV (solid line), 30.2 meV (dashed line), and 30.8 meV (dotted line). Here, $T = 250$ K.

## 4. Numerical results and discussions

The parameters used in the calculations of the absorption coefficient for specific GaAs/AlAs CQW are as follow [9–11], $\chi_\infty = 10.9,\ \chi_0 = 12.9,\ m = 0.067m_0$ ($m_0$ being the mass of free electron), $\hbar\omega_0 = 36.6$ meV. Two transitions included in numerical results are $n = 0,\ n' = 1,\ \ell = \ell' = 1$ and $n = 0, n' = 2, \ell = \ell' = 1$.

From Fig. 1 we can see that the dependence of the ACF on the intensity $E_0$ is nonlinear. The ACF increases with amplitude $E_0$ of EMW, while the photon energy rises up, their ACF decreases (Fig. 2).

Especially, in Fig. 2, each curve has two maximum peaks which are symmetric each together through the value $\hbar\Omega = \hbar\omega_0 = 36.6$ meV. The maxima appear at the photon value of $\hbar\Omega$ satisfying the condition $\hbar\Omega = \hbar\omega_0 \pm \Delta E_{n,\ell}$. Because $E_{n,\ell} = \hbar^2 B_{n,\ell}^2 \big/ (2mR^2)$, so $\Delta E_{n,\ell}$ decreases with the wire's radius $R$ increasing. Consequently, the distance between two peaks, $2\Delta E_{n,\ell}$, decreases. This result is of significant importance when we use an external electric field to measure distances between two maxima to determine the energy levels of electrons in the wire.

In Fig. 3, we can see three maxima and the peaks for each curve. This is because with any fixed value set $n, n', \ell, \ell'$, the curves have two peaks satisfying the condition $\Delta E_{n,\ell} = \hbar\omega_0 \pm \hbar\Omega$. The transition of $n = 0,\ n' = 2,\ \ell = \ell' = 1$ have more contribution than the one of $n = 0,\ n' = 1,\ \ell = \ell' = 1$. Although the transition of $n = 0,\ n' = 1,\ \ell = \ell' = 1$ results in two peaks, these contributions is less significant than the one of $n = 0,\ n' = 2,\ \ell = \ell' = 1$. The simultaneous combination of two contributions generates three peaks. The two higher peaks correspond to the transition $n = 0,\ n' = 2,\ \ell = \ell' = 1$ (more contribution). Similar to the results from Fig. 2, this result can be used to measure distances between two maxima to determine the energy levels of electrons in the wire.

## 5. Conclusion

In this paper, we have derived an analytical expression of the (nonlinear) ACF of an intensity electromagnetic field in CQW. We numerically calculated and plotted the ACF for GaAs/AlAs CQW to clarify the theoretical results. Numerical results for this CQW present clearly the dependence of the ACF on the energy $\hbar\Omega$ and amplitude $E_0$ of the field, the temperature $T$ of the system, and on the radius $R$ of a CQW.

Computational results show that the dependence of the ACF on the intensity $E_0$ is nonlinear. The importance of the present work is the appearance of resonant peaks in Figs. 2 and 3 satisfying the resonant conditions $\hbar\Omega = \hbar\omega_0 \pm \Delta E_{n,\ell}$ or $\Delta E_{n,\ell} = \hbar\omega_0 \pm \hbar\Omega$. Therefore, they can be applied to optically detect the electron spectrum in the CQW.

## References

[1] Y. Zhang et al., Science 281 (1998) 973.
[2] S. Schmitt-Rink, D.S. Chemla, D.A.B. Miller, Adv. Phys. 38 (1989) 89.
[3] N. Nishiguchi, Phys. Rev. B 52 (1995) 5279.
[4] Y.B. Yu, Sh.N. Zhu, K.X. Guo, Solid State Commun. 139 (2006) 76.
[5] N.Q. Bau, D.M. Hung, N.B. Ngoc, J. Korean, Phys. Soc. 54 (2009) 765.
[6] N.L. Kang, Y.J. Lee, S.D. Choi, J. Korean, Phys. Soc. 44 (2004) 1535.
[7] N.Q. Bau, T.C. Phong, J. Phys. Soc. Jpn. 67 (1998) 3875.
[8] M. Massale, N.C. Constantinou, Phys. Rev. B 48 (1993) 11128.
[9] J. Singh, Physics of Semiconductors and Their Heterostructures, McGraw-Hill, Singapore, 1993. p. 455.
[10] B.K. Ridley, Quantum Processes in Semiconductors, Clarendon Press, Oxford, 1993. p. 256.
[11] S.C. Lee, J.W. Kang, H.S. Ahn, M. Yang, N.L. Kang, S.W. Kim, Physica E 28 (2005) 402.