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Influence of Polaron Effects on the Optical Absorptions in Asymmetrical Quantum Wells

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Abstract: The effect of the electron-phonon interaction on the optical absorptions is theoretically studied for electrons confined in Morse quantum wells. The wave functions and energy levels are described in Morse quantum well by perturbation theory when the electron-phonon interaction is considered, and analytic expression for the optical absorption is obtained by the compact density-matrix method and the iterative procedure. The numerical results for typical GaAs/AlGaAs material show that when considering the electron-phonon interaction the optical absorption coefficients are enhanced, and the total optical absorption is strongly bleached at the linear center. It is obtained that the larger the asymmetry of the quantum wells is, the sharper the peak will be when considering the electron-phonon interaction, and the greater influence of the polaron will be. Furthermore, the correction of electron-phonon interaction effect on the energies of the electron makes the peak shift to the aspect of the high energy.

Key words: Morse quantum well; optical absorption coefficient; polaron
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1 Introduction

In the past few years, increasing interest for problems concerning the electron-phonon interaction and polaron phenomena in semiconductor systems with quantum confinement has been stimulated by the fabrication of quantum-well hetero-structures, quantum wires, nanocrystals, *etc.* [1-4]. Of particular interest is the quasi-two-dimensional optical polaron, with most emphasis being devoted to its strict two-dimensional characterization within the framework of an idealized approximation, accounting for the almost planar aspect of the electron in a thin quantum well and yet interacting with the bulk longitudinal optical (LO) phonon modes of the well material [1]. Electron-phonon interaction, particularly anharmonic ones described by the third rank polar tensors may give substantial contribution to the corresponding nonlinear optical susceptibilities, particularly in the case of low-dimensional or nonstructured materials [5].

The nonlinear phenomena connected with the intersubband transitions in some low-dimensional structures have been extensively studied both theoretically and experimentally [5-8]. Among the nonlinear optical properties, more attention has been paid to the nonlinear optical absorption mainly with considering the electron-phonon interaction effects. The common theoretical calculation of the relevant work in the literature [5,6] is that the electron interacts more effectively with the LO phonons in low dimensions and consequently certain nonlinear optical absorption coefficients scale by large factors over those obtained by ignoring the influence of electron-LO-phonon interaction. Several authors [5,6] have calculated the electron-phonon interaction effects on the nonlinear optical properties in some low-dimensional structures, but as we know, up to the present time,

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no one else has studied the optical absorption in asymmetric Morse potential considering the electron-phonon interaction. In the following, we will study the optical absorption in Morse quantum wells considering the electron-LO-phonon interaction effects.

It should be illustrated that in this paper we consider the confined electron as interacting with the bulk phonon modes merely. Since in the most commonly researched compound materials (such as GaAs, for example) the electron-phonon coupling is rather weak, an appropriate approach is to deal with the Fröhlich interaction as a perturbation. In the following we restrict our considerations only to the weak-coupling regime.

In this paper, the optical absorption coefficients in $GaAs/Al_xGa_{1-x}As$ Morse quantum wells are studied, with most emphasis being devoted to the influence of electron-phonon interaction on the optical absorption. In Section 2, the Hamiltonian, relevant wave functions and energy levels, and the analytical expression of the optical absorption are described. In Section 3, the numerical results of the absorption coefficients are presented for $GaAs/Al_xGa_{1-x}$ as Morse quantum wells. At last, brief conclusions are obtained.

2 Theory

We now consider a Morse quantum well as following [9]:

$$V(z) = U_0(1 - e^{-az})^2, \quad (-\infty < z < \infty), \tag{1}$$

where z is the real space variable, and a^{-1} is the range of the potential. The Fig. 1 in Ref. [8] shows the shape of the Morse well with several different a. And the figure reveals that the asymmetry of the Morse well increases with an decrease in the parameter a.

We consider the electron to be interacting with the optical phonons in the Morse quantum well structure. In the effective mass approximation, the Hamiltonian of the system can be written as

$$H = H_e + H_{ph} + H_{e\text{-}LO}, \tag{2}$$

where

$$H_e = \frac{\boldsymbol{P}^2}{2m^*} + \frac{p_z^2}{2m^*} + V(z), \tag{3}$$

is the electron part, here $V(z)$ is the Morse confining potential and z represents the quantum well's grown direction, and

$$H_{ph} = \sum_q \hbar\omega_{LO} a_q^+ a_q \tag{4}$$

is the phonon part, where a_q^+ and a_q are the creation and annihilation operator for the LO-phonon, respectively, ω_{LO} is the LO phonon frequency and $\hbar$ is the Planck's constant. The last term of the Eq. (2) is the Fröhlich interaction [4], which is given by

$$H_{e\text{-}LO} = \sum_q [V_q a_q \exp(i\boldsymbol{q}\cdot\boldsymbol{\rho}) \exp(iqz) + h.c.], \tag{5}$$

In the above, $(\boldsymbol{\rho}, z)$ and $(\boldsymbol{P}, p_z)$ denote the electron position and momentum. The interaction amplitude is related to the electron-phonon couple constant α and the phonon wave vector $\boldsymbol{Q} = (\boldsymbol{q}, q_z)$ through $V_q = (4\pi\alpha)^{1/2}/Q$.

The unperturbed wave equation for the electron is given by

$$H_e \Phi_{k,n}(\boldsymbol{\rho}, z) = \varepsilon_n(k)\, \Phi_{k,n}(\boldsymbol{\rho}, z), \quad n = 0, 1, 2, \cdots\cdots \tag{6}$$

where

$$\Phi_{k,n}(\boldsymbol{\rho}, z) = \varphi_n(z)\, \phi_k(\boldsymbol{\rho}), \quad n = 0, 1, 2, \cdots\cdots \tag{7}$$

So the function $\phi_k(\boldsymbol{\rho})$ and the eigenenergies $\varepsilon_n(k)$ are

$$\phi_k(\boldsymbol{\rho}) = U_c(r) \exp(i\boldsymbol{k}_\parallel \cdot \boldsymbol{\rho}), \tag{8}$$

and

$$\varepsilon_n(k) = E_n + \frac{\hbar^2}{2m^*} |k_\parallel|^2, \tag{9}$$

where $\boldsymbol{k}_\parallel$ and $\boldsymbol{\rho}$ are the wave and position vectors in the x-y plane, respectively, and $U_c(r)$ is the periodic part of the Bloch function in the conduction band at $k = 0$.

And we have

$$\left[\frac{p_z^2}{2m^*} + V(z)\right]\varphi_n(z) = E_n \varphi_n(z), \tag{10}$$

the above energy levels E_n and the corresponding wave functions are given [9],

$$E_n = \frac{\hbar^2 a^2}{2m^*}[\lambda(n + 1/2) - (n + 1/2)^2], \tag{11}$$

$$\varphi_n(z) = N(n,\lambda)\, y^{\lambda-\frac{1}{2}-n} L_n^{(2\lambda-2n-1)}(y)\exp(-y/2),$$
$$0 \leqslant n \leqslant \lambda - \frac{1}{2}, \tag{12}$$

with

$$y = 2\lambda\exp(-az), \tag{13}$$

where $L_n^{(2\lambda-2n-1)}(y)$ denote the Laguerre polynomials and the normalization constant $N(n,\lambda)$ is determined as

$$N(n,\lambda) = \left[\frac{a(2\lambda-2n-1)\Gamma(n+1)}{\Gamma(2\lambda-n)}\right]^{\frac{1}{2}}, \tag{14}$$

Since $\delta \ll 1$ (*i. e.* $\delta = 0.068$ in GaAs), we assume the electron to be almost free in the transverse directions and thus utilize a plane wave representation for its motion parallel to the x-y plane, *i. e.*, we take $\varphi_k(\boldsymbol{\rho}) \sim \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\rho})$. We begin by expressing the general total wave function in a product form of the electron and phonon parts, *i. e.*, $\psi = \Phi_{k,n}(\boldsymbol{\rho},z)\chi_{\mathrm{ph}} = \varphi_n(z)\,\phi_k(\boldsymbol{\rho})\chi_{\mathrm{ph}}$. For the ground state we take the electron to be in the lowest subband ($n=0$) and select χ_{ph} as the phonon vacuum $|0\rangle$ simply because at low temperatures ($kT \ll \hbar\omega_{\mathrm{LO}}$) there will be no effective phonons.

Since in the most commonly study for Ⅲ-Ⅴ compound (such as GaAs) the electron-phonon coupling strength is rather weak, an appropriate approach is to treat the Fröhlich interaction $H_{\text{e-LO}}$ as a perturbation. Up to first order, we have

$$|\psi_{k,n,\mathrm{ph}}\rangle = |0\rangle|\Phi_{k,n}\rangle + \sum_{Q}\sum_{k'}\sum_{n}\frac{\langle\Phi_{k',n}|\langle 1_Q|H_{\text{e-LO}}|0\rangle|\Phi_{k,0}\rangle}{\varepsilon_n(k)-\varepsilon_0(k')-\hbar\omega_{\mathrm{LO}}}|1_Q\rangle|\Phi_{k',n}\rangle, \tag{15}$$

where $|\Phi_{k,n}\rangle$ is the ground state function, $|0\rangle$ is no effective phonon function, $\varepsilon_n(k)$ and $\varepsilon_0(k')$ are the eigenenergies.

Using the same compact density-matrix approach, the linear and the third-order nonlinear absorption coefficients $\alpha^{(1)}(\omega)$ and $\alpha^{(3)}(\omega,I)$ can be obtained, respectively, by Ref [8]:

$$\alpha^{(1)}(\omega) = \omega\sqrt{\frac{\mu}{\varepsilon_{\mathrm{R}}}}\frac{|M_{ij}|^2\sigma_s\hbar\Gamma_{ij}}{\hbar^2(\omega-\omega_{ij})^2+(\hbar\Gamma_{ij})^2}, \tag{16}$$

$$\alpha^{(3)}(\omega,I) = \omega\sqrt{\frac{\mu}{\varepsilon_{\mathrm{R}}}}\left(\frac{1}{2\varepsilon_0 n_{\mathrm{r}} c}\right)\frac{\sigma_s|M_{ij}|^2\Gamma_{ij}\left[|M_{ii}-M_{jj}|^2(3\omega_{ij}^2-4\omega\omega_{ij}+\omega^2-\Gamma_{ij}^2)-4|M_{ij}|^2(\omega_{ij}^2+\Gamma_{ii}^2)\right]}{\hbar^3(\omega_{ij}^2+\Gamma_{ii}^2)\left[(\omega_{ij}-\omega)^2+\Gamma_{ij}^2\right]^2}, \tag{17}$$

where $\omega_{ij} = \dfrac{E_j - E_i}{\hbar}$ is Bohr frequency, and $M_{ij} = q\langle\Psi_j|z|\Psi_i\rangle$ is dipole matrix element ($i,j=0,1$), σ_s is the density of electron in the Morse quantum well, a is the electronic charge, I is the optical power per unit area, $\varepsilon_{\mathrm{R}} = n_{\mathrm{r}}^2\varepsilon_0$ is the real part of the permittivity, n_{r} is the refractive index, and c is the speed of light in free space.

The total absorption coefficient $\alpha(\omega,I)$ is given by

$$\alpha(\omega,I) = \alpha^{(1)}(\omega) + \alpha^{(3)}(\omega,I), \tag{18}$$

3　Results and Discussion

In the following, we will calculate the optical absorption for GaAs/AlGaAs Morse quantum wells. The parameters used in our numerical work are adopted as [10]: $\sigma_s = 5\times10^{22}\ \mathrm{m}^{-3}$, $\dfrac{1}{\Gamma_{ii}} = 1$ ps, $\dfrac{1}{\Gamma_{ij}} = 0.14$ ps, $m^* = 0.067\ m_e$ (m_e is the mass of the free electron), $\hbar\omega_{\mathrm{LO}} = 36.25$ meV, $\delta = 0.068$, $\mu = 4\pi\times10^{-7}\ \mathrm{H\cdot m^{-1}}$, $n_{\mathrm{r}} = 3.2$.

Fig. 1 illustrates the two components of the optical absorption ($\alpha^{(1)}$ and $\alpha^{(3)}$) as well as the total optical absorption ($\alpha^{(1)}+\alpha^{(3)}$) for the parameter $a = 0.83\ \mathrm{nm}^{-1}$ at an incident optical intensity of $13.5\times10^{10}\ \mathrm{W\cdot m^{-2}}$. The large positive absorption is due to the $\alpha^{(1)}$ contribution and this large absorption is significantly reduced by the third-order nonlinear $\alpha^{(3)}$ which is negative. So, the total optical absorption coefficient α is significantly reduced by the $\alpha^{(3)}$ contribution. Therefore, the third-order nonlinear optical absorption $\alpha^{(3)}$ should be considered when the incident optical intensity I comparatively strong, which can induce nonlinear absorption. However, when we take into account of the polaron effects (dotted line), the linear $\alpha^{(1)}$ of the system is over thirty percent greater than the one without considering the electron-LO-phonon interaction

(solid line), and the third-order nonlinear $\alpha^{(3)}$ is over seventy percent larger. The total optical absorption will be strongly bleached at the linear center.

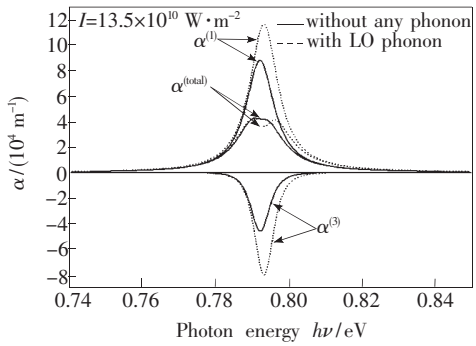

Fig. 1 The linear, third-order nonlinear and total optical absorption coefficients versus the incident photon energy $h\nu$ with the parameter $a = 0.83\ \mathrm{nm}^{-1}$ at an incident optical intensity $I = 13.5 \times 10^{10}\ \mathrm{W \cdot m^{-2}}$. For two cases: (1) considering the electron-LO-phonon interaction (dotted line); (2) without considering the electron-LO-phonon interaction (solid line).

In Fig. 2 we plot the total absorption α versus the incident photon energy $h\nu$ for the same well $a = 0.83\ \mathrm{nm}^{-1}$ for three different optical intensities: (1) $I = 0$, (2) $I = 6.0 \times 10^{10}\ \mathrm{W \cdot m^{-2}}$, (3) $I = 15.5 \times 10^{10}\ \mathrm{W \cdot m^{-2}}$. From Fig. 2 we can see that the total optical absorption coefficient will reduce strongly with the incident optical intensity I increasing. It also can been seen that with the incident optical intensity $I = 15.5 \times 10^{10}\ \mathrm{W \cdot m^{-2}}$ the polaron absorption peak will be significantly slip up into two peaks

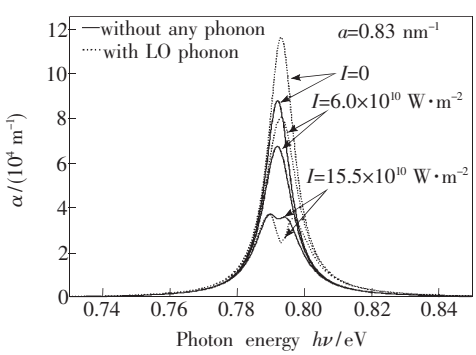

Fig. 2 The total optical absorption coefficient α versus the photon energy $h\nu$ for three different values of the incident optical intensity I with the parameter $a = 0.83\ \mathrm{nm}^{-1}$. For two cases: (1) considering the electron-LO-phonon interaction (dotted line); (2) without considering the electron-LO-phonon interaction (solid line).

(dotted line), while the total absorption is little bleached without considering the electron-LO-phonon interaction (solid line). That means the electron-phonon interaction plays an important role in the calculation of α for a Morse quantum well.

In Fig. 3, Fig. 4 and Fig. 5, the linear optical absorption $\alpha^{(1)}$, the third-order nonlinear $\alpha^{(3)}$ and the total absorption α are shown as the function of the photon energy $h\nu$ for three different values of the parameter $a = 0.83, 0.85, 0.87\ \mathrm{nm}^{-1}$ with $I = 5.0 \times 10^{10}\ \mathrm{W \cdot m^{-2}}$, respectively. From Fig. 3, Fig. 4 and Fig. 5, it can be seen that the linear, the third-order and the total absorption coefficients will increase with the parameter a increasing when we ignore the

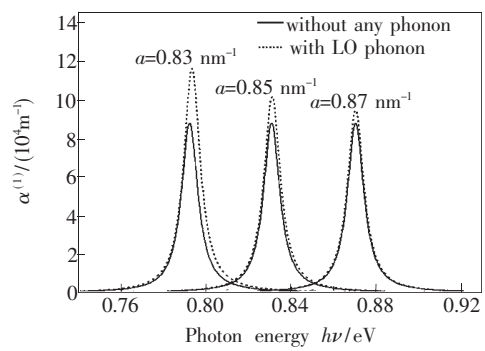

Fig. 3 The linear optical absorption coefficient $\alpha^{(1)}$ versus the photon energy $h\nu$ for three different values of the parameter a. For two cases: (1) considering the electron-LO-phonon interaction (dotted line); (2) without considering the electron-LO-phonon interaction (solid line).

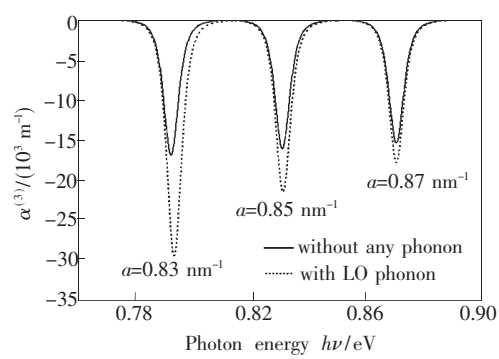

Fig. 4 The third-order nonlinear optical absorption coefficient $\alpha^{(3)}$ versus the photon energy $h\nu$ for three different values of the parameter a with the incident optical intensity $I = 5.0 \times 10^{10}\ \mathrm{W \cdot m^{-2}}$. For two cases: (1) considering the electron-LO-phonon interaction (dotted line); (2) without considering the electron-LO-phonon interaction (solid line).

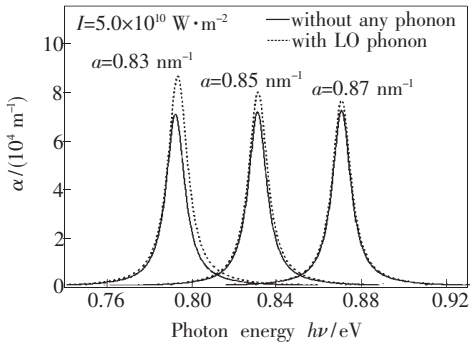

Fig. 5　The total optical absorption coefficient α versus the photon energy $h\nu$ for three different values of the parameter a with the incident optical intensity $I = 5.0 \times 10^{10}$ W · m^{-2}. For two cases (1) considering the electron-LO-phonon interaction (dotted line); (2) without considering the electron-LO-phonon interaction (solid line).

polaron effects (solid line). But when we consider the electron-LO-phonon interaction (dotted line), the linear and the total absorption coefficients will reduce significantly with the parameter a increasing. A very important feature is that the larger the asymmetry of the quantum wells is, the sharper the peak will be when taking into account of the electron-LO-phonon interaction, and the bigger influence of the polaron will be. Furthermore, the resonant peaks move a little to the aspect of the high energy for taking into account of the electron-phonon interaction (dotted line). Compared to the results in Ref. [8], our results reveal that geometric confinement has an important effect on the theoretical values of the optical absorption.

The physical explanations for the electron-phonon enhancement will be given. It is known that the LO phonon in ionic crystals involves the relative motion of positive and negative ions. This follows polarization and has a strong interaction with electromagnetic waves. So, the LO phonon has obvious influence on the optical properties of ionic crystals. Furthermore, the LO phonon has an important effect on the electron transition between the intersubband when the system has the photon radiating. Thus, when the electron-LO-phonon interaction is taken into account, the optical absorption coefficients are enhanced and the total absorption is strongly bleached at large incident optical intensity.

4　Conclusion

In conclusion, the optical absorption coefficients of the weak-coupling optical polaron systems in the Morse quantum well media are studied theoretically taking into account of the electron-LO-phonon interaction. Numerical results are illustrated for a typical GaAs/AlGaAs Morse quantum well. It is obtained that the electron-phonon interaction increases optical absorption coefficients and makes the total optical absorption strongly bleach at the linear center. A very important feature is that the larger the asymmetry of the quantum wells, the sharper the peak will be when taking into account the electron-LO-phonon interaction, and the bigger influence of the polaron will be. Furthermore, the correction of electron-phonon interaction effect on the energies of the electron makes the peak shift to the aspect of the high energy. The results are in good agreement with the experimental measurement. As we know, with recent advances in modern epitaxial growth techniques, it has become possible to fabricate such a semiconductor Morse quantum well. It is hoped that the results of the paper may be helpful for practical devices such as ultrafast optical switches and for practical exploitation of the quantum-size effect in devices.

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极化子效应对非对称量子阱中光吸收系数的影响

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摘要: 从理论上研究子电子-声子相互作用对 Morse 量子阱中光吸收系数的影响,首先利用微扰论方法求出考虑极化子效应时的电子波函数和能级,然后利用密度矩阵和迭代法得到光吸收系数的解析表达式,最后以典型的 GaAs/AlGaAs Morse 量子阱为例进行数值计算。结果表明,极化子效应使光吸收系数比仅考虑电子的情况增大了,并且在相同光强的情况下吸收饱和现象更明显; 极化子效应的影响随着阱的非对称性的增强而增大; 电声相互作用对电子能级的修正导致光吸收系数峰值向高能方向偏移。

关 键 词: Morse 量子阱; 光吸收系数; 极化子效应

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