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The second-harmonic generation susceptibility in semiparabolic quantum wells with applied electric field

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ABSTRACT

The second-harmonic generation susceptibility in semiparabolic quantum wells with applied electric field is investigated theoretically. For the same topic studied by Zhang and Xie [Phys. Rev. B 68 (2003) 235315] [1], some new and reliable results are obtained by us.

It is easily observed that the second harmonic generation susceptibility decreases and the blue shift of the resonance is induced with increasing of the frequencies of the confined potential. Moreover, a transition from a two-photon resonance to two single-photon resonances will appear adjusted by the frequencies of the confined potential. Similar results can also be obtained by controlling the applied electric field. Surprisingly, the second harmonic generation susceptibility is weakened in the presence of the electric field, which is in contrast to the conventional case. Finally, the resonant peak and its corresponding resonant energy are also taken into account.

1. Introduction

The study of the low-dimensional semiconductor quantum systems with quantum confinement, such as quantum wells (QWs), quantum wires, quantum rings and quantum dots [1–12], has attracted much attention in experimental and theoretical subject because of the enhanced nonlinear effect. To fully understand and predict experimental phenomenon, the nonlinear optical properties in these semiconductor structures, such as optical absorption and refractive index changes, second-harmonic generation (SHG), third-harmonic generation and optical rectification, have been so intensively studied theoretically [1–17]. These enhance nonlinear effects that have great potential for developing semiconductor quantum micro-device, such as high-speed electro-optical modulators, far-infrared photo detectors, and semiconductor optical amplifiers [18–21].

In the past few years, the study of the optical properties in semiconductor QWs has been so intensively studied [1–3,13–17]. This is because the nonlinear effects can be enhanced more dramatically in QWs than in bulk materials. For the bulk susceptibility, it is not very large because of the symmetry of the crystal structure. For nanomaterials also with symmetric structure, even-order nonlinear optical effects are usually vanishing in theory. Thus the contributions to the second order nonlinear optical susceptibilities are zero for a symmetrical QW, but as the symmetry is broken, nonvanishing contributions to second order nonlinear optical susceptibilities are expected to appear [2]. Consequently, in order to obtain the enhanced second order nonlinear optical susceptibilities in QWs, externally applied electric fields are used to remove the symmetry [1,2,15,16,22] or the QW structures are produced with a built-in asymmetry using advanced material growing technology [5,23,24]. Recently, Guo and Du [25] reported their results for linear and nonlinear optical absorption coefficients and refractive index changes in asymmetrical Gaussian potential QWs with applied electric field. After this moment, the other optical properties in the asymmetrical Gaussian potential QWs are investigated, such as nonlinear optical rectification [26], SHG[27], and nonlinear optical absorption via two-photon process [28]. But these are serious errors in these above reports for the optical properties in asymmetrical Gaussian potential QWs because of the replacement of the asymmetrical Gaussian potential with the semiparabolic potential under the condition of a certain limit [29]. Also, for the model of semiparabolic QWs with the electric field, some bad wavefunctions and the energy levels are chosen by those authors [25–28]. Electric field effect on the second-order nonlinear optical properties of parabolic and semiparabolic quantum wells has been reported by Zhang and Xie [1], however their results for the SHG susceptibility in electric-field-biased parabolic QWs have

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been proved to be wrong [2]. Factually, there are some serious errors reported in Ref. [1] for the SHG susceptibility in a semi-parabolic QW with an applied electric field. So it is very necessary for us to investigate the nonlinear optical properties in semi-parabolic quantum wells with applied electric field.

In this paper, the electric-field-induced SHG susceptibility in semiparabolic QWs is investigated theoretically. Also, the influence of the applied electric field and the frequencies of the confined potential on the SHG susceptibility has been taken into account. Compared with Ref. [1], the new results show that (1) the SHG susceptibility in semiparabolic QWs depend dramatically on the frequencies of the confined potential and the external electric field; (2) the SHG susceptibility decreases and the blue shift of the resonance is induced with increasing of the frequencies of the confined potential; (3) the SHG susceptibility is weakened in the presence of the electric field, which is in contrast to the conventional case. This paper is organized as follows: Hamiltonian, the relevant wave functions and energy levels are briefly described in Section 2. Also the analytical expressions of the SHG susceptibility in semiparabolic QWs are presented in this section. Numerical calculations and detailed discussions for typical $Al_xGa_{1-x}Al/GaAs$ materials are given in Section 3. Finally, a brief summary is presented in Section 4.

2. Theory

2.1. Electronic structure

Within the framework of effective-mass approximation, the Hamiltonian of an electron confined in semiparabolic QWs in the presence of electric field along the z-axis can be written as

$$H = -\frac{\hbar^2}{2m_e^*}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+V(z)+qFz. \tag{1}$$

with

$$V(z) = \begin{cases}\frac{1}{2}m_e^*\omega_0^2 z^2, & z \geq 0,\\ \infty, & z < 0,\end{cases} \tag{2}$$

where z represents the growth direction of theQWs. m_e^* is the effective mass in materials. $\hbar$ is the Planck constant, ω_0 is the frequency of the semiparabolic confined potential in QWs, F is the strength of the electric field and q is the absolute value of the electric charge. Under the envelope wave-function approximation, the eigenfunctions $\Psi_{t_n,k}(r)$ and eigenenergies $\varepsilon_{t_n,k}$ are the solutions of the Schrödinger equation for H and are given by [1,25–28]

$$\Psi_{t_n,k}(r) = \Phi_{t_n}(z)U_c(\mathbf{r}_\parallel)\exp(i\mathbf{k}_\parallel\cdot\mathbf{r}_\parallel) \tag{3}$$

and

$$\varepsilon_{t_n,k} = E_{t_n}+\frac{\hbar^2k_\parallel^2}{2m_e^*} \tag{4}$$

Here, $\mathbf{k}_\parallel$ and $\mathbf{r}_\parallel$ are respectively the wave vector and coordinate in the xy plane and $U_c(r)$ is the periodic part of the Bloch function in the conduction band at $\mathbf{k} \equiv 0$. $\Phi_{t_n}(z)$ and E_{t_n} can be obtained by solving the following Schrödinger equation:

$$H_z\Phi_{t_n}(z) = \left[-\frac{\hbar^2}{2m_e^*}\frac{\partial^2}{\partial z^2}+V(z)+qFz\right]\Phi_{t_n}(z) = E_{t_n}\Phi_{t_n}(z). \tag{5}$$

The electronic energy levels and corresponding wave functions are given as follows [1]:

$$E_{t_n} = (2t_n+1-\alpha^2\beta^2)\frac{\hbar\omega_0}{2}, \quad n = 1, 2, 3\ldots, \tag{6}$$

and

$$\Phi_{t_n}(z) = N_n\exp(-\alpha^2(z+\beta)^2)H_{t_n}(\alpha(z+\beta)), \tag{7}$$

with

$$\alpha = \sqrt{\frac{m_e^*\omega_0}{\hbar}}, \quad \beta = \frac{qF}{m_e^*\omega_0^2} \tag{8}$$

where H_{t_n} is the Hermite functions and t_n is real, N_n is the normalization constant. t_n is determined by $\Phi_{t_n}(z=0) \equiv 0$, that is to say, the relation always should be satisfied as $H_{t_n}(\alpha\beta) \equiv 0$. Obviously, $t_n = 2n+1$ as the electric field is absent, where $n = 0, 1, 2\ldots$.

2.2. The second-harmonic generation susceptibility

The formulas of the SHG susceptibility in the two models will be derived by using the compact-density-matrix method and the iterative procedure. The system is excited by electromagnetic field $\mathbf{E}(t) = \tilde{E}e^{i\omega t}+\tilde{E}e^{-i\omega t}$. Let us denote ρ as the one-electron density matrix for this regime. Then the evolution of density matrix is given by the time-dependent Schrödinger equation:

$$\frac{\partial\rho_{ij}}{\partial t} = \frac{1}{\hbar}[H_0-qz\mathbf{E}(t),\rho]_{ij}-\Gamma_{ij}(\rho-\rho^{(0)})_{ij}. \tag{9}$$

where H_0 is the Hamiltonian for this system without the electromagnetic field $\mathbf{E}(t)$; $\rho^{(0)}$ is the unperturbed density matrix; and Γ_{ij} is the relaxation rate.

Eq. (9) is calculated by the following iterative method [1,29,30]:

$$\rho(t) = \sum_n \rho^{(n)}(t), \tag{10}$$

with

$$\frac{\partial\rho_{ij}^{(n+1)}}{\partial t} = \frac{1}{i\hbar}\{[H_0,\rho^{(n+1)}]_{ij}-i\hbar\Gamma_{ij}\rho_{ij}^{(n+1)}\}-\frac{1}{i\hbar}[qz,\rho^{(n)}]_{ij}\mathbf{E}(t). \tag{11}$$

The electric polarization of the quantum system due to $\mathbf{E}(t)$ can be expressed as

$$P(t) \approx \varepsilon_0\chi_\omega^{(1)}\tilde{E}e^{i\omega t}+\varepsilon_0\chi_{2\omega}^{(1)}\tilde{E}^2e^{2i\omega t}+c.c.+\varepsilon_0\chi_0^{(2)}\tilde{E}^2, \tag{12}$$

where $\chi_\omega^{(1)}$, $\chi_{2\omega}^{(2)}$ and $\chi_0^{(2)}$ are the linear, SHG and optical rectification susceptibility respectively.

With the same compact density matrix approach and the iterative procedure as [30], the analytical expression of the SHG susceptibility is given as [1,2,22,27]

$$\chi_{2\omega}^{(2)} = \frac{q^3\sigma M_{12}M_{23}M_{31}}{\varepsilon_0}\times\frac{1}{(E_{31}-2\hbar\omega+i\hbar\Gamma_0)(E_{21}-\hbar\omega+i\hbar\Gamma_0)} \tag{13}$$

where σ is the surface density of electrons in the QWs, Γ_0 is the phenomenological relaxation rate, E_{ij} is the energy interval of two different electronic states, and M_{ij} is the off-diagonal matrix element which is given by $M_{ij} = \langle i|z|j\rangle$ where $(i, j = 1, 2, 3)$. The SHG susceptibility has a resonant peak for the condition as $\hbar\omega = E_{21} = E_{31}/2$ given by

$$\chi_{2\omega,max}^{(2)} = \frac{q^3\sigma M_{12}M_{23}M_{31}}{\varepsilon_0(\hbar\Gamma_0)^2} \tag{14}$$

3. Results and discussions

In this section, the electric-field-induced SHG susceptibility in semiparabolic quantum wells is investigated theoretically. Numerical calculations are carried out on typical $Al_xGa_{1-x}Al/GaAs$ materials. The parameters adopted in the present work are as