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Second-harmonic generation coefficients in asymmetrical semi-exponential quantum wells

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ABSTRACT

Second-harmonic generation (SHG) coefficients in asymmetrical semi-exponential quantum wells (ASEQW) are studied theoretically. The eigenfunctions and the energy eigenvalues are obtained by solving Schrödinger equation within the framework of effective mass approximation. In addition, the analytic expression of SHG coefficients is acquired by using compact-density-matrix approach and iterative method. The results show that both σ and U_0, which are parameters of the bound potential in the growth direction of ASEQW, have great influences on the magnitude and the resonant frequencies of SHG coefficients.

1. Introduction

Thanks to the rapid progress in semiconductor growth techniques in recent years, it is possible to produce low-dimensional semiconductor structures such as quantum wells, quantum wires, quantum dots and superlattices. It is well known that the decreasing dimensionality enhances the quantum confinement of carriers and results in discrete energy levels. Consequently, the confinement of carriers in low-dimensional semiconductor structures brings out novel electronic and optical properties of great interest. Therefore, it is meaningful to study the nonlinear optical properties in low-dimensional semiconductor structures.

In order to enhance second order nonlinear optical properties in low-dimensional semiconductor structures, researchers have brought forward and investigated many asymmetric structures such as asymmetrical semi-parabolic quantum wells, asymmetric coupled quantum wells and asymmetrical semi-exponential quantum wells [1–6]. In 2005 Zhang and Guo studied polaron effects on the third-order nonlinear optical susceptibility in asymmetrical semi-parabolic quantum wells [1]. In 2009, Wang et al. researched optical rectification in the asymmetric coupled quantum wells [2]. In 2012, Liu et al. investigated linear and nonlinear intersubband optical absorption and refractive index change in asymmetrical semi-exponential quantum wells [3]. Among the second nonlinear optical properties many attentions are paid to second-harmonic generation (SHG) coefficients. For instance, in 1996, Guo and Chen investigated SHG coefficients in quantum wells within electric field, and they found that SHG coefficients are influenced by both the well width and the strength of the applied electric field, in addition to the fact that the SHG coefficients enhance when the polaron effect is taken into account [4]. In 2009, Chen et al. studied the SHG coefficients in asymmetric double triangular quantum wells and concluded that sharper peaks of the SHG coefficients can be obtained, when an appropriate electric field is applied to the asymmetric double triangular quantum wells because of the double-resonant enhancement [5]. In 2010, Shao et al. discussed the SHG coefficients in cubical quantum dots with applied electric field, and they showed that the SHG coefficients are not monotonic functions neither of the length of the cubical quantum dot nor the applied electric field, but larger SHG coefficients can be acquired by selecting proper length of the cubical quantum dot and strength of electric field [6].

In this paper, we theoretically discuss the SHG coefficients in asymmetrical semi-exponential quantum wells (ASEQW). We organize the paper as follows. In Section 2, the eigenfunctions and energy eigenvalues are acquired by solving Schrödinger equation. We obtain the analytical expression of the SHG coefficients using the compact-density-matrix approach and iterative method. In Section 3, we present numerical results and some discussions. Finally, a brief conclusion is exhibited in Section 4.

2. Theory

2.1. Energy eigenvalues and eigenfunctions

In our research we consider the case that an electron is confined in ASEQW. The expression of the Hamiltonian of the system can be given as follows when the framework of effective mass approximation is taken into consideration.

$$H=-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+U(z), \tag{1}$$

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where

$$U(z)=\begin{cases}U_0(e^{z/\sigma}-1) & z\geq 0\\ \infty & z<0.\end{cases} \tag{2}$$

In the equations above z denotes the growth direction of the quantum well, $\hbar$ represents Planck constant, m^* is the effective mass of electron in conduction band, and both U_0 and σ are parameters which are determined by the property of the ASQW. Moreover, the parameters U_0 and σ have great influences on the bound potential U. The influences are exhibited in Figs. 1 and 2. From Fig. 1 it can be found that when σ is same, the value of bound potential increases with the augment of U_0 at a same point of the coordinate axis z. In contrast, we can observe from Fig. 2 that when U_0 remains unchanged, the magnitude of the bound potential decreases with increasing σ.

We suppose that the solution of Schrödinger equation is $\psi_{n,\mathbf{k}}(\mathbf{r})$ and substitute the solution into the Schrödinger equation and then we can have the following equation:

$$H\psi_{n,\mathbf{k}}(\mathbf{r})=\varepsilon_{n,\mathbf{k}}\psi_{n,\mathbf{k}}(\mathbf{r}), \tag{3}$$

where $\varepsilon_{n,\mathbf{k}}$ is the energy eigenvalue. With the method of separation of variables the solution of the Schrödinger equation can be written as

$$\psi_{n,\mathbf{k}}(\mathbf{r})=\phi_n(z)u_c(\mathbf{r})e^{i\mathbf{k}_\parallel\cdot\mathbf{r}_\parallel}, \tag{4}$$

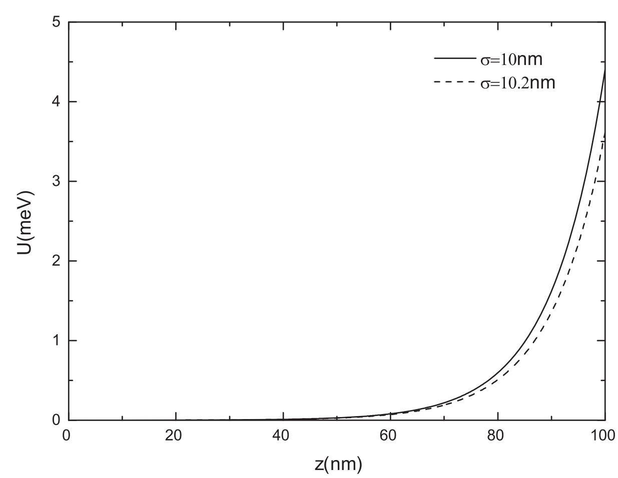

Fig. 1. The bound potential as function of z for two different values of σ, $\sigma=10$ nm and $\sigma=10.2$ nm.

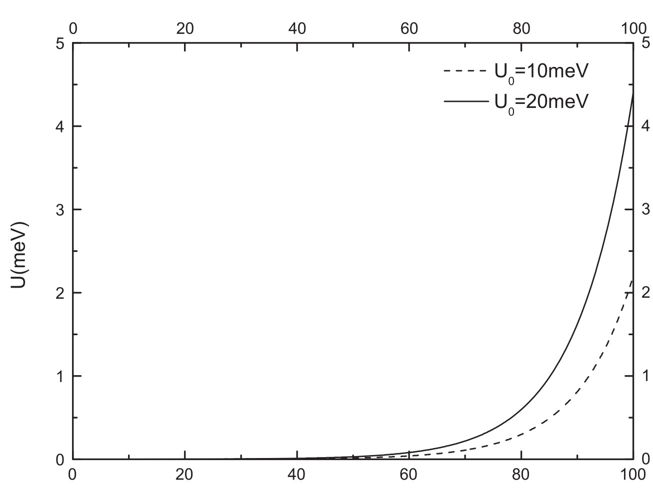

Fig. 2. The bound potential as function of z for two different values of U_0, $U_0=10$ meV and $U_0=20$ meV.

and the energy eigenvalues have the following form:

$$\varepsilon_{n,\mathbf{k}}=E_n+\frac{\hbar^2}{2m^*}\mathbf{k}_\parallel^2, \tag{5}$$

where $\mathbf{k}_\parallel$ and $\mathbf{r}_\parallel$ denote the wave vector and coordinate in the x–y plane respectively. $u_c(r)$ is the periodic part of the Bloch function in the conduction band at $\mathbf{k}=0$. $\phi_n(z)$ is the eigenfunction and E_n is the energy eigenvalue in the growth direction of the ASQW. The Schrödinger equation of the z direction is

$$H_z\phi_n(z)=E_n\phi_n(z), \tag{6}$$

where H_z represents the z part of the Hamiltonian H which can be expressed as

$$H_z=-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2}+U(z). \tag{7}$$

In order to solve Eq. (6), we assume:

$$a^2=\frac{8m^*U_0\sigma^2}{\hbar^2},\quad b=\frac{8m^*(E_n+U_0)\sigma^2}{\hbar^2},\quad \xi=ae^{z/2\sigma}. \tag{8}$$

With the above assumption the Schrödinger equation of the z direction can be rewritten as

$$\xi^2\frac{d^2\phi_n(\xi)}{d\xi^2}+\xi\frac{d\phi_n(\xi)}{d\xi}-(\upsilon^2+\xi^2)\phi_n(\xi)=0, \tag{9}$$

where $\upsilon=i\sqrt{b}$. The above equation is a modified Bessel equation whose solution can be acquired with the same method in Ref. [10]. Its solution is

$$\phi_n(\xi)=AK_\upsilon(\xi)+BI_\upsilon(\xi), \tag{10}$$

where A and B are arbitrary constants. Because $I_\upsilon(\xi)$ increases exponentially when ξ multiplies toward infinity, $I_\upsilon(\xi)$ cannot satisfy boundary conditions. Therefore, B must be 0. As a result, Eq. (10) can be simplified as

$$\phi_n(z)=AK_{i\sqrt{b}}(ae^{z/2\sigma}). \tag{11}$$

We can obtain the value of arbitrary constant A when considering normalized condition. And the energy eigenvalues E_n can be solved with numerical method [3].

2.2. Second harmonic generation coefficients

In this section, the second-harmonic generation coefficients are acquired by using the compact density matrix method and the iterative procedure. It is supposed that an electromagnetic field is applied to the system for excitation. The field vector of the applied electromagnetic field is

$$E(t)=E_0\cos(\omega t)=\tilde{E}\exp(-i\omega t)+\tilde{E}\exp(i\omega t), \tag{12}$$

where ω is the frequency of the electromagnetic field applied to the system whose polarization vector is normal to the ASEQW. Then the evolution of the density matrix operator ρ obeys the following Liouville quantum equation [7,11]:

$$\frac{\partial\rho_{ij}}{\partial t}=\frac{1}{i\hbar}[H_0-ezE(t),\rho]_{ij}-\Gamma_{ij}(\rho-\rho^{(0)})_{ij}, \tag{13}$$

where H_0 is the Hamiltonian of the system with the application of electromagnetic field $\overrightarrow{E}(t)$, $\rho^{(0)}$ is the unperturbed density matrix, and Γ_{ij} is the phenomenological relaxation rate whose generation is attributed to the interactions of the electron–phonon and electron–electron and other collision processes. In our research we select $\Gamma_{ij}=\Gamma_0=1/T_0$ when $i\neq j$ for simplification. To solve Eq. (13) we can make use of iterative method [11],

$$\rho(t)=\sum_n\rho^{(n)}(t), \tag{14}$$