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Parameters-dependent third-order nonlinear optical susceptibility for quadratic electro-optic effect in GaN/InGaN multiple quantum wells

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Abstract

Including the contribution of spin–orbit splitting, the wave functions and energy structures of $GaN/In_xGa_{1-x}N$ multiple quantum wells (MQWs) have been calculated. For the transition between valence band and conduction band, the third-order nonlinear optical susceptibility $\chi^{(3)}$ of quadratic electro-optic effect (QEOE) for the mode whose polarization is vertical to the [0 0 1] direction of the MQWs, has been calculated. The correlations between $\chi^{(3)}$ and the width of the MQWs, and the concentration of In, are obtained.

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Keywords: Quantum wells; Nonlinear susceptibility; GaN/InGaN; Interband transition; Quadratic electro-optic effect

1. Introduction

Recently, there has been an increasing focus on the nonlinear optical properties of low-dimensional quantum-confined structures, such as multiple quantum wells (MQWs), due to their potential application in optoelectronic and photonic devices [1–4]. GaN-based semiconductor materials have attracted considerable interest of people for their good properties of wide energy gap, high electron saturated drift velocity and high thermal conductivity [5–8]. For low-order nonlinear optical effects, the calculation of nonlinear optical susceptibility, which determines the nonlinear behaviors, is very important. In contrast to bulk material, the third-order nonlinear optical susceptibility of GaN/InGaN MQWs has a great enhancement due to the existence of the quantum confinement effect in one or several directions. Since the energy gap of InGaN is wide and the spin–orbit split-off energy is similar to the energy difference between valence subbands, the contribution of the spin–orbit split-off energy cannot be neglected in the calculation of the energy band structure and nonlinear optical susceptibility of GaN/InGaN MQWs, which is different from that in GaAs-based MQWs [9,10]. On the other hand, in many experiments of MQWs, only the mode, whose polarization is vertical to the [0 0 1] direction, is working, for incident laser beam is often vertical to the surfaces of samples. So for the mode with vertical polarization, including the contribution of the spin–orbit splitting, the third-order nonlinear optical susceptibility of quadratic electro-optic effect (QEOE), due to the transitions between valence band and conduction band, has been calculated with varying of the width of the MQWs and the composition of the semiconductor material.

2. Model and theory

The schematic structure of the GaN/InGaN zinc blende MQWs used in this paper is shown in Fig. 1. Potential wells are formed because the energy gap of InGaN is smaller than that of GaN. The potential barrier between two neighboring wells is wide enough so that the wave functions in the wells will not overlap and the MQWs can be treated as a single QW in the analyses.

To calculate the energy structure, there have been a lot of methods raised by different research teams. Among them,

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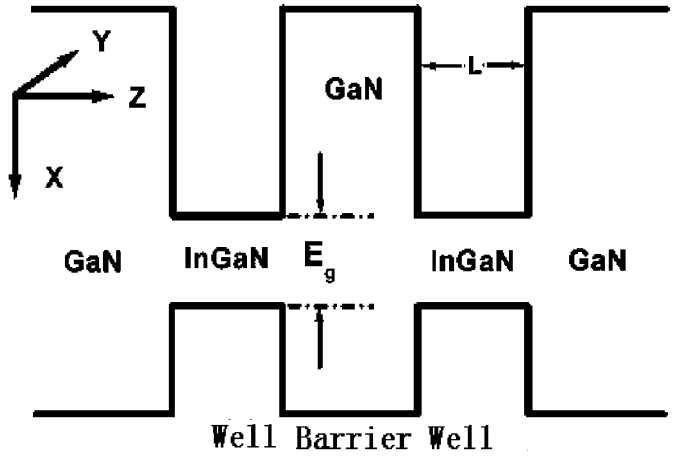

Fig. 1. The structure of GaN/InGaN multi-quantum wells.

the $k\cdot p$ method which includes the effect of all the bands (conduction and valence bands) in one Hamiltonian is quite accurate [11–13]. However, the six-band model which includes only the effect of valence bands is a good approach for wide gap semiconductors such as CdS and InGaN, because the conduction and valence bands are not strongly coupled [14]. In this paper, the six-band model is chosen for the calculation.

Using the effective mass approximation [15,16], the wave function near Γ point in the first Brillouin zone of the QW can be expanded as

$$\Psi(r)=\sum_i U_i(r)F_i(r). \tag{1}$$

Here, $F_i(\mathbf{r})$ is the slowly varying envelope function and $U_i(\mathbf{r})$ is the Bloch function. For the electrons in the conduction band, $U_i(\mathbf{r})$ equals to the ground state wave function. For the holes in the valence band, $U_i(\mathbf{r})$ corresponds to six band-edge wave functions $|V_i\rangle$ $(i=\mathrm{HH}\uparrow,\mathrm{LH}\uparrow,\mathrm{SO}\uparrow,\mathrm{SO}\downarrow,\mathrm{LH}\downarrow,\mathrm{HH}\downarrow)$. Thus, the effective mass equations of the electrons and holes can be obtained. Because the QW forms discrete quantized energy levels in the direction of z and correspondingly the electrons and holes are only confined in the z-direction, the slowly varying envelope functions can be dealt with the method of separation of variables. Setting the energy level at the top of the valence band as zero, the slowly varying envelope function and energy for the electrons at the bottom of the conduction band can be written as

$$F_c(k_x,k_y,k_z)=\frac{1}{\sqrt{L_xL_y}}\exp[i(k_xx+k_yy)]\times\sqrt{\frac{2}{L}}\sin\frac{n\pi z}{L}, \tag{2}$$

$$E_c=E_g+\frac{\hbar^2(k_x^2+k_y^2)}{2m_e^*}+\frac{\hbar^2n^2\pi^2}{2m_e^*L^2}, \tag{3}$$

where $n=1,\ 2,\ 3,\ \ldots.$ E_g is the energy gap of the semiconductor material InGaN. m_e^* is the effective mass of the electrons. L is the width of the QW. The normalization constants L_x and L_y denote the lengths of the QW in the direction of x and y, respectively. For the holes in the valence band, the Hamiltonian can be expressed as the 6×6 Luttinger-Kohn matrix H_0 [17,18]:

$$H_0(k_x,k_y,k_z)=\begin{bmatrix} A_+ & C & \frac{i}{\sqrt{2}}C & -i\sqrt{2}B & B & 0\\ C^* & A_- & -\frac{i}{\sqrt{2}}(A_+-A_-) & i\sqrt{\frac{3}{2}}C & 0 & b\\ -\frac{i}{\sqrt{2}}C^* & \frac{i}{\sqrt{2}}(A_+-A_-) & -\Delta+\frac{1}{2}(A_++A_-) & 0 & i\sqrt{\frac{3}{2}}C & i\sqrt{2}B\\ i\sqrt{2}B^* & -i\sqrt{\frac{3}{2}}C^* & 0 & -\Delta+\frac{1}{2}(A_++A_-) & \frac{i}{\sqrt{2}}(A_+-A_-) & \frac{i}{\sqrt{2}}C\\ B^* & 0 & -i\sqrt{\frac{3}{2}}C^* & -\frac{i}{\sqrt{2}}(A_+-A_-) & A_- & -C\\ 0 & B^* & -i\sqrt{2}B^* & -\frac{i}{\sqrt{2}}C^* & -C^* & A_+ \end{bmatrix}. \tag{4}$$

Here, Δ denotes the splitting of spin–orbit coupling. A_+, A_-, B and C have the forms

$$\begin{aligned} A_\pm &= -\frac{\hbar^2}{2m_0}[(k_x^2+k_y^2)(\gamma_1\pm\gamma_2)+k_z^2(\gamma_1\mp2\gamma_2)],\\ B &= -\frac{\sqrt{3}\hbar^2}{2m_0}[\gamma_2(k_x^2-k_y^2)-i2\gamma_3k_xk_y],\\ C &= \frac{\sqrt{3}\hbar^2}{m_0}\gamma_3(ik_x+k_y)k_z, \end{aligned} \tag{5}$$

where m_0 is the real mass of the electrons. γ_1, γ_2 and γ_3 are Luttinger parameters.

Then, the envelope wave function of the holes in the z-direction can be expanded by the wave functions of infinite square potential well as follows:

$$F_v^i(z)=\sqrt{\frac{2}{L}}\sum_{m=1}^{M}C_i^m\sin\frac{m\pi z}{L}. \tag{6}$$

Here, i denotes one of the six band-edge wave functions and $i=\mathrm{HH}\uparrow,\mathrm{LH}\uparrow,\mathrm{SO}\uparrow,\mathrm{SO}\downarrow,\mathrm{LH}\downarrow,\mathrm{HH}\downarrow$. In this way, the effective mass equation of the holes can be rewritten into an eigenvalue problem of a $6\,\mathrm{M}\times6\,\mathrm{M}$ matrix