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High Second-Order Nonlinear Susceptibility Induced in GaN/$Al_xGa_{1-x}N$ Coupled Quantum Well for Infrared Photodectors Application

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The second harmonic generation (SHG) of GaAs/$Al_xGa_{1-x}As$ a wurtzite coupled quantum wells (CQWs) is studied theoretically for different widths of well, barrier and values Al concentration, taking into account the strain-induced piezoelectric (PZ) effects. The analytical expression of the SHG susceptibility is deduced by using the compact density matrix approach. The confined wave functions and energies of electrons GaN/Al_xGA_{1-x} N are calculated in the effective-mass approximation, solving the Schrödinger equation by Numerov's method using six order approximations for the derivatives. The calculated results also reveal that by adjusting the widths of well, the barrier and Al concentration respectively, a set of optimal structural parameters can be found for obtaining a strong SHG susceptibility.

Keywords: Second-harmonic generation, Wurtzite quantum well, Strain-induced piezoelectric, Density matrix approach, Numerov method.

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1. INTRODUCTION

Recently, there has been a considerable interest in interband transitions (IBTs) in nitride semiconductor quantum well (QW) structures [1-5]. These heterostructures are characterized by very large conduction-band offsets (up to about 1.75 eV) allowing for ISBT at record short wavelengths in the near-infrared spectral region. At the same time, they feature especially fast ISBT relaxation lifetimes due to the highly polar nature of (Al)(Ga)N. The spontaneous and piezoelectric polarizations of these structures [6] can give rise to large polarization sheet charges on the interfaces or surfaces of the system, which, in turn, create a definite internal built-in electric field (BEF) inside the heterostructure. This property is ideally well suited to the development of ultrafast all-optical modulators and switches operating at fiber-optic communication wavelengths.

In this paper, we show that the built-in electric fields induced by the piezoelectricity and spontaneous polarization in a wurtzite GaN/$Al_xGa_{1-x}N$ QW breaks the symmetry of the confinement potential profile and leads to large second-order susceptibilities. In particular, $\gamma^{(2)}$ was investigated as a function of Al content, well width, barrier width and pump photo energy. The organization of this paper is as follows. In Section 2, theory and model are presented. The model of calculation used in this paper is based on using the effective mass Schrödinger with the Numerov numerical technique which we provide. Simulation results of our models and discussions are illustrated in Section 3. In this section, our results have been explained and show that the proposed structure is a better model for applications in microwave and optical switches. Finally, the paper contains a short conclusion.

2. THEORY AND MODEL

The second-order susceptibilities $\chi_{2\omega}^{(2)}$ can be expressed by

$$\chi_{2\omega}^{(2)} = \frac{q^3 n}{\varepsilon_0 \hbar^2} \sum_{m,n} \langle z_{ln} \rangle \langle z_{nm} \rangle \langle z_{nl} \rangle \times \Big\{ \frac{1}{(\omega - \Omega_{nl} - i\gamma_{nl})(2\omega - \Omega_{ml} - i\gamma_{ml})} + \frac{1}{(\omega - \Omega_{nl} - i\gamma_{nl})(2\omega + \Omega_{ml} - i\gamma_{ml})} - \frac{1}{(\omega - \Omega_{ml} - i\gamma_{ml})} + \frac{1}{(\omega - \Omega_{nl} - i\gamma_{nl})} \times \frac{1}{(\omega - \Omega_{mn} - i\gamma_{mn})} \Big\},$$

where $\langle z_{ij} \rangle$ is $\langle \varphi_i | z | \varphi_j \rangle$, $E_i - E_j/\hbar$, $1/\gamma_{ij}$ is the dephasing times, and q the electronic charge. It can be easily checked that this expression is nonzero only for asymmetric wave functions. In order to calculate the χ^2, the eigenenergies and envelope wave function should be obtained. One solves the effective-mass Schrödinger equation:

$$-\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2}\varphi(z) + V(z)\varphi(z) = E\varphi(z),$$

where m^* the the effective mass of the particle, and the conduction band nonparabolicity has been neglected, and $V(z)$ the conduction band offset given by

$$V(z) = \Delta E^c + eF_z z,$$

where ΔE^c is the conduction band discontinuity between the well and barrier layers in the absence of strain, and F_z is the sum of the spontaneous (zero strain) and piezoelectric (strain-induced) field, which is given by

$$F^{Al_xGa_{1-X}N} = -\frac{\left(P_{SP}^{Al_xGa_{1-X}N} + P_{PE}^{Al_xGa_{1-X}N} - P_{SP}^{GaN}\right)L_b}{\varepsilon_0\left(2\varepsilon_e^{GaN}L_w + \varepsilon_e^{Al_xGa_{1-X}N}L_b\right)}$$

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$$F^{GaN} = 2\frac{\left(P_{SP}^{Al_xGa_{1-X}N} + P_{PE}^{Al_xGa_{1-X}N} - P_{SP}^{GaN}\right)L_w}{\varepsilon_0\left(2\varepsilon_e^{GaN}L_w + \varepsilon_e^{Al_xGa_{1-X}N}L_b\right)}$$

where P_{SP}^x and P_{PE}^x respectively denote the spontaneous and the piezoelectric polarization of layer x (x = GaN, AlxGa$_{1-x}$N) ε_e is the dielectric constant of materiel x, and Lw and Lb respect the widths of the GaN well-layer and AlxGa$_{1-x}$N barrier layer. Under the effective mass and envelope wave-function approximation, the electronic eigen-function are expressed by

$$\varphi(z)\begin{cases} a_1\exp(\rho z) & z\langle \\ a_2\exp i(kz) + a_3\exp -i(kz) \\ a_4\cosh(\rho z) + a_5\sinh(\rho z) \end{cases}$$

where $\hbar^2\rho^2 = 2m_b^*(V_b - E)$ and $\hbar^2k^2 = 2m_w^*E$. The eigen-energy E_n of the double quantum well in z-direction can be numerically solved by standarded boundary condition of electronic bound state.

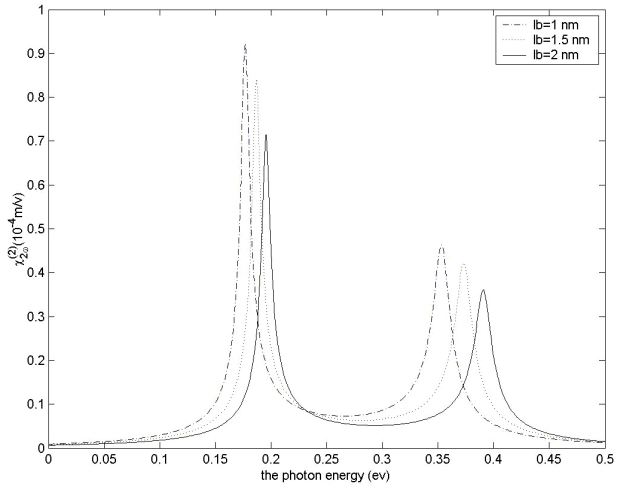
3. NUMERICALS RESULTS AND DISCUSSIONS

In order to find the optimal parameters of size structure for obtaining strong SHG coefficient in the wurtzite nitride DQW, the numerical calculations on a GaN AlxGa$_{1-x}$N DQW are performed in the present section. Material parameters and values of polarization and elastic constants used in the calculation are given in Table 1 [7].

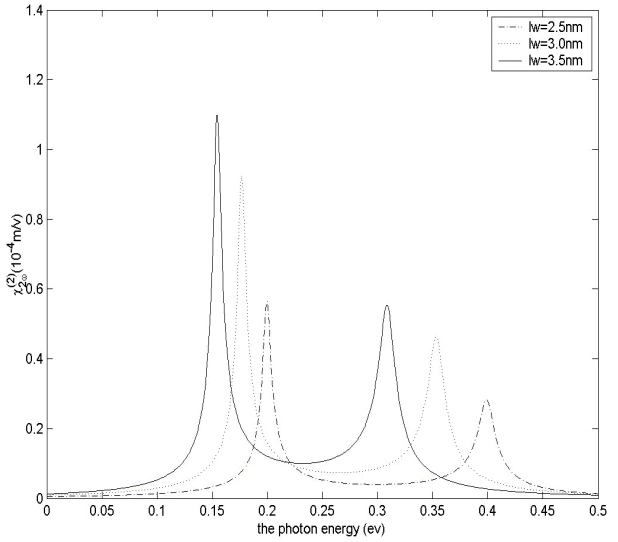
	GaN	$Al_xGa_{1-x}N$
$a(A^0)$	3.189	$3.122\,x + 3.189(1-x)$
ε_r	10	$8.5\,x + 10(1-x)$
$e_{31}(C/m^2)$	-0.490	$-0.600\,x - 0.490(1-x)$
$e_{33}(C/m^2)$	0.730	$-1.460\,x + 0.730(1-x)$
$C_{13}(GPa)$	103	$108\,x + 103(1-x)$
$C_{13}(GPa)$	373	$405\,x + 373(1-x)$
$P_{sp}(C/m^2)$	-0.029	$-0.081\,x - 0.029(1-x)$

Taking $\Delta E_c = 2$ eV as conduction band discontinuity and $\gamma_{12} = \gamma_{23} = \gamma = 0.006emV$, $m_{GaN}^* = 0.33m_0$, $m_{GaN}^* = \left[0.33x + 0.22(1-x)\right]m_0$, is the mass of a free electron, the sheet density $n = 2 \times 10^{12}$ cm^{-2}.

Using Numerov's method for the numerical solution of the Schrödinger equation (Eq.(4)) in one dimension, we find both for the eigenvalue and the wavefunction. The efficiency of Numerov's method lies in the fact that one obtains a local error of $O(h^6)$ with just one evaluation of V and E per step. This should be compared to the Runge–Kutta algorithm that needs six function evaluations per step to achieve a local error of $O(h^6)$. Fig. 1. shows the second harmonic generation (SHG) coefficients function of the pump photon energy $\hbar\omega$. The well-width L_w, the barrier-width L_b and doped concentration x are parameters in Fig. 1(a), (b) and (c), respectively. It can be seen from the figure that, the strength of the SHG coefficient in the CQW achieves the magnitude of 10^{-4} m/V, which is one to two orders higher than that in GaN/AlGaN single quantum well [8]. The strong SHG effect is primarily ascribed to the large dipole-matrix elements in nitride DQW. Moreover, it is observed from



a



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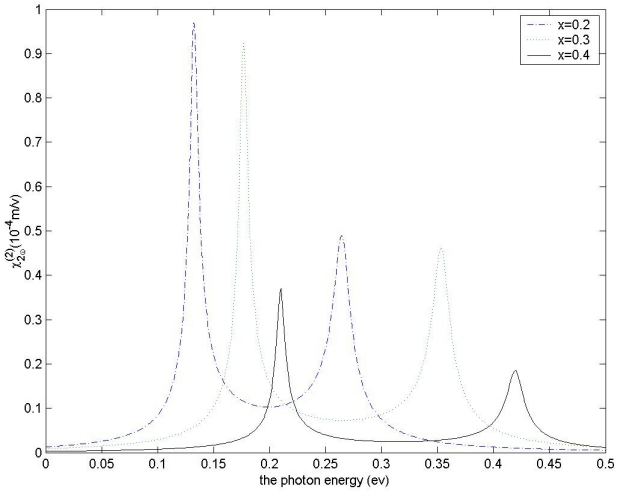

c

Fig. 1 – SHG coefficients $\chi^{(2)}$ 2ω as a function of the photon energy $\hbar\omega$ for different parameters of well-width L_w (L_b = 1 nm, x = 0.3 in (a)), the barrier-width L_b (L_w = 3 nm, x = 0.3 in (b)) and the doped-concentration x (L_w = 3 nm, L_b = 1 nm in (c))

Fig. 1(a) that, with the increase of the well-width L_w, the SHG coefficients increases apparently, and the resonant photon frequencies have a obvious red-shift. For example, as L_w increases from 2.5 to 3.5 nm, the SHG coefficients increase nearly three times, and the resonant photon frequencies $\hbar\omega$ decrease. Hence it is an effective method that the DQW with relatively large L_w should be chosen for obtaining large SHG. On the other hand, the no table red-shift of the pump photon frequencies should also be taken into account. When the barrier-width L_b is over 2.0 nm (Fig. 1(b)) and the doped concentrate $x = 0.2$ (Fig. 1(c)), with the decreases of L_b or x, the SHG coefficient also increases remarkably. Moreover, the resonant photon frequencies $\hbar\omega$ have obviously blue-shift. The strong strength characteristics of the SHG susceptibility can be attributed to the complicated competitive relationships between the effect of strong built-in electric fields (F^{AlGaN} and F^{GaN}) and the quantum size effect of the DQWs (the well-width L_w and barrier width L_b) [9,10]. Indeed, with the increase of L_w, the size confinement of the CQW for the carrier becomes weaker and weaker. But the built-in electric field F^{GaN} in GaN-barrier becomes larger [14, 15], which leads to stronger confined effect to the DQW systems. On the other hand, as the barrier-width L_b increases, the quantum-size confined effect for the carrier in QW will decrease. But the built-in electric field F^{AlGaN} in the AlGaN -well region becomes stronger with the creases of L_b, which enhances the confined effect to the carrier in the DQW. Hence these integrated factors strongly influence the distributions of electronic wave-functions and eigen-energy, which affects the magnitude of the dipole-matrix elements at last. This is quite beneficial to getting strong SHG coefficients in nitride wurtzite DQWs.

In conclusion, the second-order nonlinear optical susceptibilities of GaN/$Al_xGa_{1-x}N$ DQW by taking into account influences of polarization field have been performed in this paper, and a Numerov numerical technique to solve Schrödinger equation is used. A large value of $\chi^{(2)}$ (several orders than that of bulk GaN) has been obtained. In addition, $\chi^{(2)}$ as functions of well width, barrier width, Al content and pump photo energy are also given, which can provide the structure parameters to optimize $\chi^{(2)}$ of DQW. Based on the present results, we hope that the important infrared photodetectors, near infrared laser amplifiers and can be constructed based on the group- III nitride QWs.

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