

Optical Susceptibility of Third Order Harmonic Generation in A Strained $B_xGa_{1-x}N/BN$ Nano-Well

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Abstract— Wide band gap group III-N materials are given due attention for the huge potential applications for fabricating novel opto-electronic devices. Boron nitride and Gallium nitride materials are considered to be the promising wide band gap candidates ranging from the ultraviolet to the visible regions of the spectrum. In the present work, the binding energy of a hydrogenic donor and the third order susceptibility of third order harmonic generation are discussed in a $B_xGa_{1-x}N/BN$ quantum well. The barrier material is taken as GaN semiconductor whereas the Boron nitride material acts as inner well material. The energy eigen value and thereby the hydrogenic binding energy are obtained using variational technique within a single band effective mass approximation. The nonlinear optical property is investigated using density matrix method. The results can be applied for short wavelength optical devices.

Keywords- Opto-electronic devices, Susceptibility, Hydrogenic binding energy, Density matrix.

I. INTRODUCTION

Group III nitride wide band gap semiconducting materials, in general, have a high melting point, high thermal conductivity and transparency to a large spectrum. These materials can be used for short-wavelength light-emitting diodes, laser diodes and optical detectors and high electron mobility transistors [1]. Group III nitride heterostructures have huge spontaneous and piezoelectric polarization. Boron nitride is found to be in the hexagonal phase with the zinc-blende structure and it is hard material [2].

II. THEORETICAL FORMULISM

Hamiltonian of the hydrogenic impurity confined in a $B_xGa_{1-x}N/BN$ quantum well, within the framework of effective mass approximation, can be written as

$$H = -\frac{\hbar^2}{2m_e^*(E)} \nabla^2 - \frac{e^2}{\epsilon r} + V(z) \quad (1)$$

where r is the distance between the electron and the impurity, $r = \sqrt{\dots^2 + z^2}$, $m_e^*(E)$ is the energy dependent effective mass of the electron, ϵ is the dielectric constant of the BGaN material. And, $V(z)$ is the barrier height of the quantum well.

The trial wavefunction of the hydrogenic donor is chosen as

$$\Psi(r) = N \mathcal{E}(z) \exp(-\Gamma \dots^2 - zS^2) \quad (2)$$

where N is the normalization constant. The above equation describes the correlation of the electron-hole relative motion. Γ and S are the variational parameters responsible for the in plane correlation and the correlation of the relative motion in the z -direction respectively.

The hydrogenic binding energy of the donor is defined as

$$E_b = E_0 - \langle H(\Gamma, S) \rangle_{\min} \quad (3)$$

Where $\langle H(\Gamma, S) \rangle_{\min}$ is obtained by minimizing the Hamiltonian (Eq.(1)) with respect to the variation parameter.

The Schrödinger equation is solved variationally by finding $\langle H(\Gamma, S) \rangle_{\min}$ and the binding energy of the donor

in a quantum well is given by the difference between the energy with and without the Coulomb interaction. E_0 is the eigenvalue of the Hamiltonian without the Coulomb interaction term.

The nonlinear susceptibility due to the electron Raman scattering is given by [3]

$$t_{SS}^3(\check{S}_{out}, \check{S}_p, \check{S}_s, -\check{S}_p) = \frac{-2i \cdot e^4 |\langle E_i | \vec{r} | E_f \rangle|^4}{\nu_f \hbar^3 [i(\check{S}_i - 2\check{S}_s + \check{S}_p) + \Gamma][i(\check{S}_p - \check{S}_s) + \Gamma]} \times \left[\frac{1}{i(\check{S}_i - \check{S}_s) + \Gamma} + \frac{1}{i(\check{S}_p - \check{S}_i) + \Gamma} \right] \quad (4)$$

where the line broadening, $\Gamma = 1/\tau$, is the relaxation rate for states i and f and $\hbar\check{S}$ is the photon energy. \check{S}_i and \check{S}_s are the pump and emitted photon frequency respectively. The ground state energies and the first excited states are taken in order to have optical transitions assuming the selection rule, $\Delta l = \pm 1$.

III. RESULTS AND DISCUSSION

The subband energy of the electron in the conduction band in the Boron based Group-III-nitride semiconductor is computed taking into the geometrical confinement. Numerical computations are done variationally. They hydrogenic donor binding energy is obtained by assuming a trial wave function. Third order susceptibility of third harmonic generation with the photon energy is carried out. The atomic units have been followed in the determination of electronic charges and wave functions in which the electronic charge and the Planck's constant have been assumed as unity.

Fig.1 shows the variation of third-order susceptibility of third harmonic generation as a function of incident photon energy with and without the donor impurity in a $B_{0.2}Ga_{0.8}N/BN$ quantum well width 50 Å with $\hbar\check{S}_0 = 50$ meV. It is noticed that the third order susceptibility of third order harmonic generation has two peaks for both the cases, with and without adding impurity. It is also observed that the magnitude of the resonant peak suffers blue shift when the donor impurity is included in the Hamiltonian. It is well known that the relaxation time has more influence on the third-order susceptibility, hence the magnitude of the third-order susceptibility is found to be higher for longer relaxation time. And hence, the damping factor decides the lifetime of the excitons in the confined states [4]. Eventually, the relaxation time has more influence on the third-order susceptibility of third harmonic generation.

In summary, the energy eigen values, the hydrogenic binding energies, and the third order susceptibility of generation of third harmonic as a function of photon energy in a $B_xGa_{1-x}N/BN$ quantum well have been investigated taking into consideration of geometrical confinement and strain effects due to piezo-electric polarization. The Boron alloy content is taken as $x=0.2$ throughout the calculations. The large optical nonlinearities are associated with intraband transition.

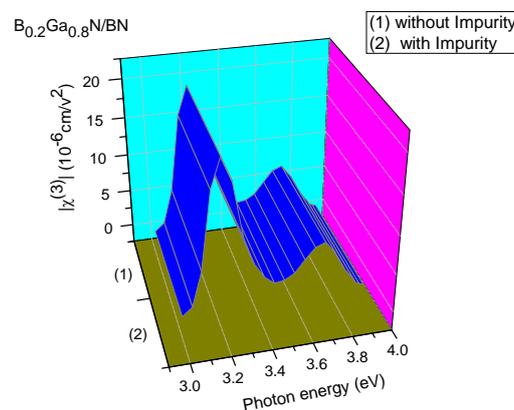


Fig.1 Variation of third-order susceptibility of third harmonic generation as a function of incident photon energy in a $B_xGa_{1-x}N/BN$ quantum well.

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