

# Pressure induced nonlinear optical properties in a strained $\mathrm{Zn}_{0.1} \mathrm{Mg}_{0.9} \mathrm{Se} /$ $\mathrm{Zn}_{0.8} \mathrm{Mg}_{0.2} \mathrm{Se} / \mathrm{Zn}_{0.1} \mathrm{Mg}_{0.9}$ Se quantum well <br> J.Abraham Hudson Mark ${ }^{1}$ and A.John Peter ${ }^{2^{*}}$ <br> ${ }^{1}$ Department of Physics, SSM Institute of Engineering and Technology, Dindigul-624 002, India. <br> ${ }^{2}$ Department of Physics, Govt.Arts and Science College, Melur-625 106. Madurai. India. 

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#### Abstract

Pressure induced exciton binding energy, optical transition energy, second order optical rectification coefficient and the third order harmonic generation of third order susceptibility are computed in $\mathrm{Zn}_{0.1} \mathrm{Mg}_{0.9} \mathrm{Se} / \mathrm{Zn}_{0.8} \mathrm{Mg}_{0.2} \mathrm{Se} / \mathrm{Zn}_{0.1} \mathrm{Mg}_{0.9}$ Se quantum well. The effects of geometrical confinement and the contribution from the induced strain are included in the Hamiltonian. The effects of internal electric field comprising spontaneous and piezoelectric polarization are considered throughout the calculations. Exciton binding energies, in the presence of hydrostatic pressure, are computed using single band effective mass approximation. Calculations are done employing the variational method and the density matrix method. The second order optical rectification coefficient and the third order susceptibility with the incident photon energy are calculated in the presence of hydrostatic pressure. It is observed that the effect of pressure has influence on the nonlinear optical properties in the Mg based ZnSe quantum well.


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## Introduction

II-VI materials are interesting due to the potential applications in novel wide spectrum optical, electronic and optoelectronic devices including light emitting diodes, laser diodes and photo-detectors. ZnSe semiconductor has been given due attention due to its wide band gap of 2.7 eV and it can be applied for fabricating potential devices [1,2] in which the emission wavelength in the range of 450 nm and 600 nm can be obtained. Nonlinear optical properties dominate in the wide band gap semiconductors. High efficiency radiative lift time is the main reason for using this material in fabricating devices [3]. Quantum dots having discrete energies, these optical properties are expected to enhance further. Ternary and quartanery materials with tailoring their physical properties and lattice constants by adjusting the constituent elements achieve the desired mechanism in order to meet out today's commercial requirements including blue diode lasers, LEDs, flat panel displays laser printing, compact displays, data storage devices, solar cells and sensor applications. Mg based ZnSe ternary alloy semiconductors are known to be very famous for fabricating devices in the visible and UV region $[4,5]$ and can be applied for cladding and wave guiding layers due to its wide direct band gap[6]. These direct band gap zincblende type II-VI materials are considered to be the promising semiconductors for realizing short wavelength efficient light emitting diode displays and laser diodes. Moreover, they are realized with the highly $n$ and $p$ type doping [7].

The application of hydrostatic pressure is considered to be an important tool to study the electronic properties in any heterostructures [8]. The pressure has a lot of influence on the electronic and optical properties of any low dimensional semiconductor system. The pressure tuning strain results the alteration of heavy hole energy level occurs the phase transition eventually. The properties of excitons in $\mathrm{ZnSe} / \mathrm{ZnMgSe}$ quantum well grown by molecular beam epitaxy have been studied and found that these properties have been enhanced due to heavy-hole-light-hole coupling in the tensile strained wells [9]. In general, blue green laser diodes based on ZnSe semiconductors are achieved and the efficiency can be improved when of these lasers are incorporated with the ZnMgSSe as cladding layer [10]. The band gap of ZnMgSe can be tuned upto high band gap around 3.6 eV by adjusting Mg alloy content [11].

Optical studies of ZnSe quantum well with ZnMgSSe Barrier and the exciton binding energies, the resonant frequency, oscillator strength, and exciton line damping. radiative and nonradiative damping rates have been presented by Platonov et al., [12]. Optical

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characterization of Mg based ZnSe mixed crystals by high pressure Bridgman method has been studied earlier [13]. The efficient carrier injection of CdSe nanocrystals incorporated $\mathrm{ZnSe} / \mathrm{ZnMgSe}$ quantum wells has been accomplished recently [14].

In the present work, the exciton binding energies, optical transition energies and some nonlinear optical properties in the presence of hydrostatic pressure in a $\mathrm{Zn}_{0.1} \mathrm{Mg}_{0.9} \mathrm{Se} / \mathrm{Zn}_{0.8} \mathrm{Mg}_{0.2} \mathrm{Se} / \mathrm{Zn}_{0.1} \mathrm{Mg}_{0.9}$ Se quantum well are carried out taking into account the spatial confinement effects and the strain contributions. The variational formulism is employed to investigate the above properties. The second order optical rectification coefficient and the third order susceptibility as a function of incident photon energy are found in the presence of pressure. The theoretical model is presented in Section 2 and the results and discussion are obtained in Section 3. Finally, the main conclusions are shortened in the last Section.

## Model And Theory

A confined exciton is considered in a $\mathrm{Zn}_{0.1} \mathrm{Mg}_{0.9} \mathrm{Se} / \mathrm{Zn}_{0.8} \mathrm{Mg}_{0.2} \mathrm{Se} / \mathrm{Zn}_{0.1} \mathrm{Mg}_{0.9} \mathrm{Se}$ quantum well in the presence of hydrostatic pressure. The confining potential is taken as zero inside the well and $\mathrm{V}_{0}$ outside. The Hamiltonian of the exciton in the strained $\mathrm{Zn}_{0.8} \mathrm{Mg}_{0.2} \mathrm{Se} / \mathrm{Zn}_{0.1} \mathrm{Mg}_{0.9}$ Se quantum well can be written as,

$$
\begin{align*}
\mathrm{H}_{\mathrm{exc}}= & -\frac{\mathrm{h}^{2}}{2 \mu_{\|}(\mathrm{p})}\left[\frac{1}{\rho_{\mathrm{j}}} \frac{\partial}{\partial \rho_{\mathrm{j}}}\left(\rho_{\mathrm{j}} \frac{\partial}{\partial \rho_{\mathrm{j}}}\right)+\frac{1}{\rho_{\mathrm{j}}^{2}} \frac{\partial^{2}}{\partial \phi_{\mathrm{j}}^{2}}\right]-\frac{\mathrm{h}^{2}}{2 \mathrm{~m}_{\mathrm{e}}^{*}(\mathrm{p})} \frac{\partial^{2}}{\partial \mathrm{z}^{2}}-\frac{\mathrm{h}^{2}}{2 \mathrm{~m}_{\mathrm{h} \perp}^{*}(\mathrm{p})} \frac{\partial^{2}}{\partial \mathrm{z}^{2}}+\mathrm{V}_{\mathrm{j}}\left(\mathrm{z}_{\mathrm{j}}, \mathrm{p}\right) \\
& \pm \mathrm{eFz}_{\mathrm{j}}-\frac{\mathrm{e}^{2}}{\varepsilon \mathrm{r}} \tag{1}
\end{align*}
$$

where $\mathrm{j}=\mathrm{e}$ and h denote the electron and hole, respectively, $\rho_{j}$ is the in-plane co-ordinates of electron (hole), $\mu_{\|}(p)$ is the pressure dependent reduced mass of the exciton, $\mathcal{E}$ is the dielectric constant of the inner material $(\varepsilon=9.277), V_{j}\left(z_{j}, p\right)$ is the pressure related band offset confinement potential in conduction (valence) band which includes the contribution from the strain effect $\left(\mathrm{V}_{\mathrm{c}(\mathrm{v}) \text { strain }}\right)$. The values of conduction band and valence band offsets are taken from Ref.15. p is the applied hydrostatic pressure in GPa. e is the absolute value of electron charge, the effective mass of electron along the growth direction and $r=\sqrt{\rho^{2}+\left(z_{e}-z_{h}\right)^{2}}$. The sign + for the electron and - for hole with F is the built-in internal field due to the spontaneous and piezoelectric polarizations in the $\mathrm{Zn}_{0.8} \mathrm{Mg}_{0.2} \mathrm{Se}^{2} / \mathrm{Zn}_{0.1} \mathrm{Mg}_{0.9} \mathrm{Se}$ quantum structure. The reduced mass in the $\mathrm{x}-\mathrm{y}$ plane is given by

$$
\begin{equation*}
\mu_{\|}(\mathrm{p})=\frac{\mathrm{m}_{\mathrm{e}}^{*}(\mathrm{p}) \mathrm{m}_{\mathrm{h} \|}(\mathrm{p})}{\mathrm{m}_{\mathrm{e}}^{*}(\mathrm{p})+\mathrm{m}_{\mathrm{h} \|}(\mathrm{p})} \tag{2}
\end{equation*}
$$

Assuming the mass of the electron as isotropic and hence $m_{e \|}^{*}(p)=m_{e \perp}^{*}(p)=m_{e}^{*}(p)$. The hole masses are determined from the Luttinger parameters $\gamma_{1}$ and $\gamma_{2}$ which are expressed as [16]

$$
\begin{align*}
& \frac{1}{\mathrm{~m}_{\mathrm{h} \perp}}=\frac{1}{\mathrm{~m}_{0}}\left(\gamma_{1}-2 \gamma_{2}\right)  \tag{3}\\
& \frac{1}{\mathrm{~m}_{\mathrm{h} \|}}= \frac{1}{\mathrm{~m}_{0}}\left(\gamma_{1}+\gamma_{2}\right) \tag{4}
\end{align*}
$$

where $m_{0}$ is the free electron mass.
The shifts in energy of conduction band and valence band due to the strain effects are computed as shown below. The shift of electron and hole bands are determined by the elastic stiffness constants. The pressure dependent strain-induced potential for the conduction band with the influence of Mg - incorporation is given by [17]

$$
\begin{equation*}
\mathrm{V}_{\text {Cstrian }}(\mathrm{x}, \mathrm{p})=\mathrm{a}_{\mathrm{c}}\left[\varepsilon_{\mathrm{xx}}(\mathrm{x}, \mathrm{p})+\varepsilon_{\mathrm{yy}}(\mathrm{x}, \mathrm{p})+\varepsilon_{\mathrm{zz}}(\mathrm{x}, \mathrm{p})\right] \tag{5}
\end{equation*}
$$

where $\mathrm{a}_{\mathrm{c}}$ is the deformation potential constant of conduction band, $\varepsilon_{x x}(x, p)=\varepsilon_{y y}(x, p)=\varepsilon_{\|}(x, p)=\frac{a_{0}(x, p)-a(x, p)}{a_{0}(x, p)}$ where $a_{0}(x, p)$ and $a(x, p)$ are the pressure and Magneisum dependent lattice parameters of bulk ZnSe and MgSe respectively. The change in length is occurred as the ZnSe has a smaller bond length than MgSe. And $\varepsilon_{z z}(x, p)=\varepsilon_{\perp}(x, p)=-2 \frac{C_{12}(x, p)}{C_{11}(x, p)} \varepsilon_{\|}(x, p)$, the values of parameters $\mathrm{C}_{11}(\mathrm{x}, \mathrm{p})$ and $\mathrm{C}_{12}(\mathrm{x}, \mathrm{p})$ are shown in Table 1.

Table 1. Material parameters* used in the calculations

| Parameter | $\mathbf{Z n S e}$ | $\mathbf{M g S e}$ | $\mathbf{Z n}_{0.8} \mathbf{M g}_{0.2} \mathbf{S e}$ | $\mathbf{Z n}_{0.1} \mathbf{M g}_{0.9 \mathbf{S e}}$ |
| :---: | :---: | :--- | :--- | :--- |
| $m_{e}^{*}$ | 0.114 | 0.202 | 0.131 | 0.193 |
| $\gamma_{1}$ | 3.94 | 2.84 | 3.826 | 2.951 |
| $\gamma_{2}$ | 1 | 0.43 | 0.942 | 0.485 |
| $\varepsilon$ | 9.4 | 8.2 | 9.277 | 8.319 |
| $a(\mathrm{~nm})$ | 0.567 | 0.591 | 0.569 | 0.589 |
| $\mathrm{C}_{11}(\mathrm{GPa})$ | 8.57 | 7.58 | 8.471 | 7.677 |
| $\mathrm{C}_{12}(\mathrm{GPa})$ | 5.07 | 4.86 | 5.049 | 4.881 |
| $\mathrm{a}(\mathrm{eV})$ | 1.65 | -1.0 | 1.38 | -0.743 |
| $\mathrm{~b}(\mathrm{eV})$ | -1.8 | -1.27 | -1.747 | -1.323 |
| $E_{g}^{\mathrm{r}}(\mathrm{eV})$ | 2.719 | 4 | 2.815 | 3.872 |

*Ref. [30]

Thus, the pressure dependent strain-induced potential for the valence band with the incorporation of Mg in ZnSe which can be written as [18]
$\mathrm{V}_{\mathrm{Vstrain}}(\mathrm{x}, \mathrm{p})=\mathrm{a}_{\mathrm{v}}\left[\left(\varepsilon_{\mathrm{xx}}(\mathrm{x}, \mathrm{p})+\varepsilon_{\mathrm{yy}}(\mathrm{x}, \mathrm{p})+\varepsilon_{\mathrm{zz}}(\mathrm{x}, \mathrm{p})\right)-\frac{\mathrm{b}}{2}\left(\varepsilon_{\mathrm{xx}}(\mathrm{x}, \mathrm{p})+\varepsilon_{\mathrm{yy}}(\mathrm{x}, \mathrm{p})-2 \varepsilon_{\mathrm{zz}}(\mathrm{x}, \mathrm{p})\right]\right.$
where $a_{v}$ and $b$ are the deformation potential constants of valence band.
The pressure dependent electron (hole) confinement potential, $V\left(\rho, z_{j}, p\right)$, due to the band offset in the $\mathrm{Zn}_{0.8} \mathrm{Mg}_{0.2} \mathrm{Se} /$ $\mathrm{Zn}_{0.1} \mathrm{Mg}_{0.9} \mathrm{Se}$ quantum well structure is given by
$V\left(z_{j}, p\right)= \begin{cases}0 & \left.\left.\left|z_{j}\right|<L\right) p\right) / 2 \\ V_{0} & \left|z_{j}\right| \geq L(p) / 2\end{cases}$
where $\mathrm{L}(\mathrm{p})$ is pressure dependent well width and $\mathrm{V}_{0}$ is expressed as

$$
\begin{equation*}
V_{0}=Q_{c} \Delta E_{g} \tag{8}
\end{equation*}
$$

where $\mathrm{Q}_{\mathrm{c}}$ is the conduction band offset parameter and the $\Delta E_{g}$ is the band gap of inner quantum well. Taking into account the band gap discontinuity to the $\mathrm{Zn}_{0.8} \mathrm{Mg}_{0.2} \mathrm{Se}$ quantum well, the distribution between the conduction band and valence band is taken as $70: 30$ [19].
Thus, the total strain induced band gap is given by

$$
\begin{equation*}
\Delta \mathrm{E}_{\mathrm{g}}(\mathrm{x})=\Delta \mathrm{E}_{\mathrm{g}}+\delta \mathrm{E}_{\mathrm{HH}}(\mathrm{x}) \tag{9}
\end{equation*}
$$

where the nonlinear variation of the band gap energy ( $\Delta E_{g}$ ) in ternary alloy ( $Z n_{1-x} M g_{. x} S e$ ) is taken as [20]

$$
\begin{equation*}
\Delta \mathrm{E}_{\mathrm{g}}=\mathrm{E}_{\mathrm{g}}(\mathrm{ZnSe})+1.37 \mathrm{x}+0.47 \mathrm{x}(\mathrm{x}-1) \tag{10}
\end{equation*}
$$

and

$$
\begin{equation*}
\delta \mathrm{E}_{\mathrm{HH}}(\mathrm{x}, \mathrm{p})=\frac{1}{3} \Delta_{0}-\left(\mathrm{a}_{\mathrm{c}}-\mathrm{a}_{\mathrm{v}}\right)\left(\frac{2 \mathrm{C}_{12}(\mathrm{x}, \mathrm{p})}{\mathrm{C}_{11}(\mathrm{x}, \mathrm{p})+\mathrm{C}_{12}(\mathrm{x}, \mathrm{p})}+2\right)\left(\frac{\mathrm{a}_{0}(\mathrm{x}, \mathrm{p})-\mathrm{a}(\mathrm{x}, \mathrm{p})}{\mathrm{a}(\mathrm{x}, \mathrm{p})}\right) \tag{11}
\end{equation*}
$$

The polarization in a self formed wurzite quantum well consists of spontaneous and piezoelectric components out of which the latter has three independent nonvanishing components [21]. Subsequently, the total polarization is the addition of spontaneous polarization and the piezoelectric polarization in the absence of the external electric field.

The stress induced piezo electric field ( $P^{P Z}$ ) related to mismatch between the well and the barrier material along the z direction is given by

$$
\begin{equation*}
\mathrm{P}^{\mathrm{PZ}}(\mathrm{x}, \mathrm{p})=\mathrm{e}_{31}(\mathrm{x}, \mathrm{p})\left(\varepsilon_{\mathrm{xx}}(\mathrm{x}, \mathrm{p})+\varepsilon_{\mathrm{yy}}(\mathrm{x}, \mathrm{p})\right)+\mathrm{e}_{33}(\mathrm{x}, \mathrm{p}) \varepsilon_{z z}(\mathrm{x}, \mathrm{p}) \tag{12}
\end{equation*}
$$

where $\varepsilon_{x x}(x, p), \varepsilon_{y y}(x, p)$ and $\varepsilon_{z z}(x)$ are the strain elements in $\mathrm{Zn}_{0.8} \mathrm{Mg}_{0.2}$ Se layers as defined earlier. Thus the piezoelectric polarization is given by

$$
\begin{equation*}
\mathrm{P}^{\mathrm{PZ}}(\mathrm{x}, \mathrm{p})=2 \varepsilon_{\mathrm{xx}}(\mathrm{x}, \mathrm{p})\left(\mathrm{e}_{31}(\mathrm{x}, \mathrm{p})-\varepsilon_{33}(\mathrm{x}, \mathrm{p}) \frac{\mathrm{C}_{13}(\mathrm{x}, \mathrm{p})}{\mathrm{C}_{33}(\mathrm{x}, \mathrm{p})}\right) \tag{13}
\end{equation*}
$$

where $\mathrm{e}_{\mathrm{ij}}$ is the piezoelectric constants. Thus the total pressure induced internal fields within the quantum well and the barrier are given by [22]

$$
\begin{gather*}
\mathrm{F}_{\text {well }}(\mathrm{p})=\left|-\frac{\left(\mathrm{P}_{\mathrm{SP}(\mathrm{ZnSe})}+\mathrm{P}_{\mathrm{PE}(\mathrm{ZnSe})}-\mathrm{P}_{\mathrm{SP}(\mathrm{ZnMgSe})}\right) \mathrm{L}_{\mathrm{ZnMg}}(\mathrm{p})}{\varepsilon_{0}\left(2 \varepsilon_{\mathrm{e}(\mathrm{MgZnSe})} \mathrm{L}_{(\mathrm{ZnSe})}+\varepsilon_{\mathrm{e}(\mathrm{ZnSe})} \mathrm{L}_{(\mathrm{ZnMgse})}(\mathrm{p})\right)}\right|  \tag{14}\\
\mathrm{F}_{\text {barrier }}(\mathrm{p})=2\left|\frac{\left(\mathrm{P}_{\mathrm{SP}(\mathrm{ZnSe})}+\mathrm{P}_{\mathrm{PE}(\mathrm{ZnSe})}-\mathrm{P}_{\mathrm{SP}(\mathrm{ZnMgSe})}\right) \mathrm{L}_{\mathrm{ZnMgSe}}(\mathrm{p})}{\varepsilon_{0}\left(2 \varepsilon_{\mathrm{e}(\mathrm{ZnMgSe})} \mathrm{L}_{(\mathrm{ZnSe})}+\varepsilon_{\mathrm{e}(\mathrm{ZnSe})} \mathrm{L}_{(\mathrm{ZnMgSe})}(\mathrm{p})\right)}\right| \tag{15}
\end{gather*}
$$

where $\varepsilon_{0}$ is the dielectric constant of the respective material. Here, $\varepsilon_{e}$ is the electronic dielectric constant of material, $P_{S P Z n S e}, P_{P Z M_{g} S e}$ and $P_{S P Z n M_{g} S e}$ are the spontaneous polarizations and piezoelectric polarizations of ZnSe and the spontaneous polarization of ZnMgSe respectively. The above values can be generally calculated by the polarity of the crystal and the strains of the quantum nanostructure. Since the wurtzite crystal lattice of ZnSe and MgSe lack inversion symmetry, the heterostructure will have spontaneous polarization ( $\mathrm{P}_{\mathrm{SP}}$ ) and the piezo electric polarization $\left(\mathrm{P}_{\mathrm{PZ}}\right)$ due to strain caused by the lattice mismatch between ZnSe and MgSe material.

We have chosen the trial wave function for the exciton ground state, within the variational scheme. We take the problem of an exciton in a $\mathrm{Zn}_{0.8} \mathrm{Mg}_{0.2} \mathrm{Se}^{/} / \mathrm{Zn}_{0.1} \mathrm{Mg}_{0.9} \mathrm{Se}$ quantum well within the single band effective mass approximation, it is necessary to use a variational approach to calculate the eigen function and eigen value of the Hamiltonian and to calculate the bound exciton ground state energy. Considering the correlation of the electron-hole relative motion, the trial wave function can be chosen as,

$$
\begin{equation*}
\Psi\left(\bar{r}_{e}, \bar{r}_{h}\right)=N f_{e}\left(\rho_{e}, z_{e}\right) f_{h}\left(\rho_{h}, z_{h}\right) e^{-\alpha \rho^{2}} e^{-\beta z^{2}} \tag{18}
\end{equation*}
$$

where N is the normalization constant, $f_{e}$ and $f_{h}$ are ground state solution of the Schrödinger equation for the electrons and holes in the absence of the Coulomb interaction. The above equation describes the correlation of the electron-hole relative motion. $\alpha$ and $\beta$ are variational parameters responsible for the in-plane correlation and the correlation of the relative motion in the z -direction respectively. By matching the wave functions and the effective mass and their derivatives at boundaries of the quantum well and along
with the normalization, we fix all the constants except the variational parameters. So the wave function Eq.(18) completely describes the correlation of the electron-hole relative motion.

The Schrödinger equation is solved variationally by finding $\langle H\rangle_{\min }$ and the binding energy of the exciton in the quantum dot is given by the difference between the energy with and without Coulomb term. First, we concentrate on the calculation of the electronic structure of the $\mathrm{Zn}_{0.8} \mathrm{Mg}_{0.2} \mathrm{Se} / \mathrm{Zn}_{0.1} \mathrm{Mg}_{0.9}$ Se quantum well system for various Mg alloy content by calculating its subband energy (E) and subsequently the exciton binding energy. To calculate the ground-state energies of the heavy excitons, we minimize the expectation values of the Hamiltonian (Eq.(1)) calculated using a trial function with two variational parameters (Eq.(18)). Then, by using the density matrix approach, within a two-level system approach, the explicit expression for the nonlinear optical properties such as the nonlinear optical rectification is computed in saturation limit. The dependence of the nonlinear optical processes on the dot sizes is investigated with the different photon energy.
The pressure dependent binding energy of the excitonic system is defined as

$$
\begin{equation*}
\mathrm{E}_{\mathrm{exc}}(\mathrm{x}, \mathrm{p})=\mathrm{E}_{\mathrm{e}}(\mathrm{p})+\mathrm{E}_{\mathrm{h}}(\mathrm{p})-\left\langle\mathrm{H}_{\mathrm{exc}}\right\rangle_{\min } \tag{19}
\end{equation*}
$$

where $\mathrm{E}_{\mathrm{e}, \mathrm{h}}$ is the sum of the pressure related free electron and the free hole self-energies in the same quantum well.
The pressure dependent optical transition energy $\mathrm{E}_{\mathrm{ph}}(\mathrm{p})$ associated with the exciton is calculated using the following equation

$$
\begin{equation*}
\mathrm{E}_{\mathrm{ph}}(\mathrm{p})=\mathrm{E}_{\mathrm{e}}(\mathrm{p})+\mathrm{E}_{\mathrm{h}}(\mathrm{p})+\mathrm{E}_{\mathrm{g}}^{\Gamma}(\mathrm{x}, \mathrm{p})-\mathrm{E}_{\mathrm{exc}}(\mathrm{p}) \tag{20}
\end{equation*}
$$

where $\mathrm{E}_{\mathrm{e}}(\mathrm{p})$ and $\mathrm{E}_{\mathrm{h}}(\mathrm{p})$ are the pressure dependent confinement energies of the electron and hole respectively. $E_{g}^{\Gamma}(x, p)$ is the Magnesium and pressure dependent band gap energy of $\mathrm{Zn}_{1-\mathrm{x}} \mathrm{Mg}_{\mathrm{x}}$ Se material ( $\mathrm{x}=0.2$ ) as given in Eq.(10).

The linear susceptibility is expressed as

$$
\begin{equation*}
\chi_{0}^{1}=\frac{\sigma_{\mathrm{s}}\left|\mathrm{M}_{12}\right|^{2}}{\Delta \mathrm{E}-\mathrm{h} \omega-\mathrm{ih} \Gamma_{12}} \tag{21}
\end{equation*}
$$

The second order nonlinear optical rectification coefficient is given by [23,24]

$$
\begin{equation*}
\chi_{0}^{2}=\frac{\mathrm{q}^{3} \sigma_{\mathrm{s}} \mu_{01}^{2} \delta_{01}}{\varepsilon_{0}} \frac{2 \Delta \mathrm{E}^{2}}{\left[(\Delta \mathrm{E}-\mathrm{h} \omega)^{2}+\left(\mathrm{h} \Gamma_{0}\right)^{2}\right]\left[(\Delta \mathrm{E}+\mathrm{h} \omega)^{2}+\left(\mathrm{h} \Gamma_{0}\right)^{2}\right]} \tag{22}
\end{equation*}
$$

where $\sigma_{s}$ is the electron density in the quantum dot, $\varepsilon_{0}$ is the vacuum permittivity, $\Gamma=1 / \tau$ is the relaxation rate for states 1 and 2 and $\eta \omega$ is the photon energy. The Matrix element, $\mu_{01}=\left\langle\psi_{0}\right| z\left|\psi_{1}\right\rangle$ is defined as the electric dipole moment of the transition from the ground state $\left(\psi_{0}\right)$ to the first excited state $\psi_{1}$ with $\delta_{01}=\left\langle\psi_{1}\right| z\left|\psi_{1}\right\rangle-\left\langle\psi_{0}\right| z\left|\psi_{0}\right\rangle . \Delta E$ is the absorption energy from $\psi_{0}$ to $\psi_{1}$. We have taken the relaxation rate as 1 ps and the electron density is taken as $1 \times 10^{24} \mathrm{~m}^{-3}$.

The third-order nonlinear optical susceptibility $\chi(3)$ related to optical mixing between two incident light beams with different frequencies $\left(\omega_{1}\right.$ and $\left.\omega_{2}\right)$ is expressed as $[25,26]$

$$
\begin{gather*}
\chi^{3}\left(-2 \omega_{1}+\omega_{2} ; \omega_{1},-\omega_{2}\right)=-\frac{2 \mathrm{iNe}^{4}|\mu|^{4}}{\varepsilon_{0} \mathrm{~h}^{3}} \frac{1}{\left[\mathrm{i}\left(\omega_{0}-2 \omega_{1}+\omega_{2}\right)+\Gamma\right]\left[\mathrm{i}\left(\omega_{2}-\omega_{1}\right)+\Gamma\right]} \\
{\left[\frac{1}{\left[\mathrm{i}\left(\omega_{0}-\omega_{1}\right)+\Gamma\right]}+\frac{1}{\left[\mathrm{i}\left(\omega_{2}-\omega_{1}\right)+\Gamma\right]}\right]} \tag{23}
\end{gather*}
$$

where $\mu$ refers the dipole matrix element, defined as the transition frequency is given by $\omega_{0}=\left(E_{f}-E_{i}\right) / \eta, \mathrm{N}$ is the number of charge carriers.

## Results and discussion

Nonlinear optical properties are concentrated in a strained $\mathrm{Zn}_{0.8} \mathrm{Mg}_{0.2} \mathrm{Se} / \mathrm{Zn}_{0.1} \mathrm{Mg}_{0.9} \mathrm{Se}$ quantum well in the presence of hydrostatic pressure values using compact density formulism. The built-in internal electric fields including the spontaneous and piezoelectric polarizations are taken into consideration in the calculations. Since the heavy hole mass is common in all the experimental research works, we have taken the heavy hole mass throughout the calculations. The atomic units are used in the determination of electronic energies in which the electron charge, Planck's constant are assumed to be unit. The values of used parameter values are listed in Table. 1 and the corresponding interpolated values are also given.

The variation of exciton binding energies as a function of well width in the presence of hydrostatic pressure in a $\mathrm{Zn}_{0.1} \mathrm{Mg}_{0.9} \mathrm{Se} /$ $\mathrm{Zn}_{0.8} \mathrm{Mg}_{0.2} \mathrm{Se} / \mathrm{Zn}_{0.1} \mathrm{Mg}_{0.9}$ Se quantum well is presented in Fig.1. The effect of built in-internal field has been included in the calculation which consists of spontaneous polarization and piezoelectric polarization terms. Since the material taken in the problem is a polar semiconductor the effects of built in-internal fields play a vital role. The exciton binding energies are found to increase when the well width is reduced. Further, it is found that it reaches a maximum value for a critical well width and then starts decreasing when the well width is still decreased for all the hydrostatic pressure values [27]. It is because the quantum size effect dominates when the spatial confinement is increased. It results the enhancement of Coulomb interaction between the electron and hole and eventually, the electron (hole) wave function is compressed in the stronger confinement region. Exciton binding energy increases with the hydrostatic pressure due to the additional confinement. Further, we would like to point out that the exciton binding energy becomes the bulk value of the barrier material for the larger well width.


Fig 1. Variation of exciton binding energies as a function of well width in a $\mathbf{Z n}_{0.8} \mathbf{M g}_{0.2} \mathbf{S e} / \mathbf{Z n}_{0.1} \mathbf{M g} g_{0.9} S e q u a n t u m$ well for various hydrostatic pressure values

Pressure induced optical transition energy as a function of well width is shown in a $\mathrm{Zn}_{0.1} \mathrm{Mg}_{0.9} \mathrm{Se}^{2} / \mathrm{Zn}_{0.8} \mathrm{Mg}_{0.2} \mathrm{Se}^{2} / \mathrm{Zn}_{0.1} \mathrm{Mg}_{0.9} \mathrm{Se}$ quantum well in Fig.2. It is observed that the optical transition energy increases as the well width is decreased for all the pressure values. This is due to the confinement of electron-hole with respect to the z-plane when the well width is reduced. . The geometrical confinement effect has drastic effects on both the ground state exciton energy and the optical transition energy. The conduction band shifts under hydrostatic strain to increase the band gap. This representation obviously clearly exhibits the effects of quantum confinement [28].

In Fig.3, the variation of second order nonlinear coefficient as a function of incident energy for a confined exciton for various pressure values of a $40 \AA \mathrm{Zn}_{0.1} \mathrm{Mg}_{0.9} \mathrm{Se} / \mathrm{Zn}_{0.8} \mathrm{Mg}_{0.2} \mathrm{Se} / \mathrm{Zn}_{0.1} \mathrm{Mg}_{0.9}$ Se quantum well is displayed. It is found that the resonant peak is found to shift towards higher energies when the hydrostatic pressure is enhanced. This is because the exciton binding energy enhances with the pressure and the barrier height increases with the hydrostatic pressure. The magnitude of the pressure induced
resonant peak of nonlinear optical rectification is found to be around $10^{-4} \mathrm{~m} / \mathrm{V}$ [30]. This strong value is due to the existence of larger dipole matrix elements in the wide band gap semiconductors. Further, it is observed that that the variation of magnitude of absorption coefficient increases when the hydrostatic pressure is increased. It is because the spacing between the energy levels increases due to the pressure and reduction of well width. Further, the exciton binding energy increases when the well width is decreased. Thus there occurs a competition between the energy interval and the dipole matrix element which determines these features. The resonant frequencies are important and it should be taken into account in studying the optical properties of exciton in the low dimensional semiconductor nanostructures.


Fig 2. Variation of optical transition energy as a function of well width in a $\mathbf{Z n}_{0.8} \mathbf{M g}_{0.2} \mathbf{S e} / \mathbf{Z n}_{0.1} \mathbf{M g}_{0.9} S e q u a n t u m$ well in the presence of various hydrostatic pressure values


Fig 3. Variation of second order nonlinear rectification coefficient as a function of incident photon energy of a confined exciton for various pressure values in a $40 \AA \mathbf{Z n}_{0.8} \mathbf{M g}{ }_{0.2} \mathbf{S e} / \mathbf{Z n}_{0.1} \mathbf{M g}_{0.9}$ Se quantum well
Fig. 4 shows the variation of third-order susceptibility of third harmonic generation as a function of incident photon energy of a confined exciton in the presence of hydrostatic pressure in a $\mathrm{Zn}_{0.8} \mathrm{Mg}_{0.2} \mathrm{Se} / \mathrm{Zn}_{0.1} \mathrm{Mg}_{0.9} \mathrm{Se}$ quantum well width $40 \AA$ with $\eta \omega_{0}=50$ meV . It is observed that the third order susceptibility has two peaks and the effect of hydrostatic pressure makes the resonant peak towards higher energies (blue shift). The resonant peaks occur two times. Further, it is noted that the magnitude of the resonant peak
moves towards the higher energies with the increase of pressure values. And hence, it is concluded that the external perturbation has more influence on the resonant peak of third order susceptibility of third harmonic generation. It is observed from the figure that the relaxation time has more influence on the third-order susceptibility. The magnitude of the third-order susceptibility is found to be higher energies for longer relaxation time. The damping factor decides the lifetime of the excitons in the confined states [29]. Hence it is concluded that the relaxation time has more influence on the third-order susceptibility of third harmonic generation.


Fig 4. Variation of third-order susceptibility of third harmonic generation as a function of incident photon energy of a confined exciton in the presence of hydrostatic pressure in a $\mathbf{Z n}_{0.8} \mathbf{M g}_{0.2} \mathbf{S e} / \mathbf{Z n}_{0.1} \mathbf{M g}_{0.9}$ Se quantum well

In conclusion, the pressure induced heavy hole exciton binding energies in a $\mathrm{Zn}_{0.1} \mathrm{Mg}_{0.9} \mathrm{Se} / \mathrm{Zn}_{0.8} \mathrm{Mg}_{0.2} \mathrm{Se} / \mathrm{Zn}_{0.1} \mathrm{Mg}_{0.9} \mathrm{Se}$ quantum well have been computed taking into consideration of spatial confinement. The pressure related optical transition energy as a function of well width has been found. The optical rectification coefficient and the third-order susceptibility of third harmonic generation with the photon energy have been studied. It is observed that the resonant peaks of the interband optical spectra shift towards the blue region when the pressure is enhanced. It is believed that the investigated theoretical results on Mg based ZnSe semiconducting nanostructures are of great interests in fabricating short wavelength devices.

## References

1.T. Kummell, G. Bacher, A. Forchel, G. Lermann, W. Kiefer, B. Jobst, D. Hommel, G. Landwehr, Phys. Rev. B 57 (1998) 15439.
2. J.A. Tuchman, I.P. Herman, Phys. Rev. B 45 (1992) 11929.
3. V. Kishore, V. K. Saraswat, N. S. Saxena, Bull. Mater. Sci., 28 (2005) 431.
4. M. Strassburg, O. Schulz, U.W. Pohl, D. Bimberg, S. Itoh, K. Nakano, and A. Ishibashi, Electron. Lett. 36 (2000) 44.
5. S. O. Ferreira, H. Sitter, R. Krump, W. Faschinger, G. Brunthaler, and J. Sadowski, Semicond. Sci. Technol. 10 (1995) 489.
6. B. Derkowska , Z. Essaidi, B. Sahraoui, A. Marasek, F. Firszt and M. Kujawa, Opt.Mat.31(2009)518.
7. R. L. Gunshor and A. V. Nurmikko, MRS Bulletin 20 (1995) 15.
8.Z.Z. Guo, X.X. Liang and S.L. Ban, Physics Letters A 306 (2002) 160.
9. J. Puls, M. Rabe, A. Siarkos, and F. Henneberger, Phys.Rev.B 57 (1998) 14749.
10. David B. Laks and Sokrates T. Pantelides, Phys.Rev.B. 51 (1995) 2570.
11. M.Sohel, X.Zhou, H.Lu, M. Noemi Perez-Paz ,Maria Tamargob and Martin Muñoz, Journal of Vacuum Science \& Technology B 23 (2005) 1209.
12. A. V. Platonov, V. P. Kochereshko, D. R. Yakovlev, U. Zehnder, W. Ossau, W. Faschinger and G. Landwehr, Phys.Sol.Stat. 40 (5) (1998) 745 .
13. H. P. Hsu, P. J. Huang, C. T. Huang, Y. S. Huanga, F. Firszt, S. ŁJgowski, H. MJczyńska, K. Strzałkowski, A. Marasek and K. K. Tiong, J.Appl.Phys. 103 (2008) 013501.
14. E M Larramendi, O Schöps, M V Artemyev, D Schikora, K Lischka and U Woggon, Nanotechnology 24 (2013) 435202.
15. J.Abraham Hudson Mark and A. John Peter, In Press, J of Semiconductors.
16. R. T. Senger and K. K. Bajaj, Phys. Rev. B 68, 205314(2003).
17. J. Singh. Optoelectronics: An Introduction to Materials and Devices (New Delhi: Tata McGraw Hill: 1996)
18. G. L. Bir , E. Pikus, Symmetry and Strain-Induced Effects in Semiconductors (New York : Wiley: 1974)
19. B.König, U. Zehnder, D.R. Yakovlev, W. Ossau, T. Gerhard, M.Keim, A. Waag, and G. Landwehr, Phys. Rev. B 60, 2653 (1999).
20. M.T. Litz, M. Korn, H. Ress, U. Lunz, W. Ossau, A. Waag, G. Landwer, K. Watanabe, T. Walter, and B. Neubauer, J. Cryst. Growth 159, 54 (1996)
21. P. Prete,N. Lovergine, L. Tapfer and A.M. Mancini, Optical Materials, 17, 207(2001).
22. M.Yano et al., JCG301-302 353(2007).
23. F. Bernardini, V. Fiorentini, D. Vanderbilt, Phys. Rev. Lett. 79 (1997) 3958.
24. S. Baskoutas, E. Paspalakis, A.F. Terzis, Phys. Rev. B 74 (2006) 153306.
25. C.M. Duque, M.E. Mora-Ramos, C.A. Duque, Superlattices and Microstructures 49 (2011) 264.
26. T. Takagahara, Phys. Rev. B 36 (1987) 9293.
27. R.Sangeetha and A.John Peter, Elixir Nuclear \& Radiation Phys. 64 (2013) 19071.
28. Ansheng Liu, S.-L. Chuang, C.Z. Ning, Appl. Phys. Lett. 76 (2000) 333.
29. S.Shao, K.X.Guo, Z.H.Zhang, N.Li and C.Peng, Superlatt Microstruct. 48 (2010) 541.
30. Sadao Adachi, Properties of Semiconductor alloys: Group-IV, III-V and II-VI Semiconductors, John Wiley \& Sons Ltd, 2009.

