TÜBİTAK

Turkish Journal of Physics

http://journals.tubitak.gov.tr/physics/

Research Article

Turk J Phys
(2015) 39: 114 – 121

doi:10.3906/fiz-1407-25

Polaron effects on the second-harmonic generation in asymmetrical semiexponential quantum wells

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Received: 28.07.2014 • **Accepted/Published Online:** 25.05.2015 • **Printed:** 30.07.2015

Abstract: Polaron effects on the second-harmonic generation (SHG) in asymmetrical semiexponential quantum wells (ASEQWs) are investigated theoretically. By using the framework of the compact-density-matrix approach and iterative method, the analytical expression of the SHG coefficients in ASEQWs is presented. Numerical results are illustrated for a typical GaAs/AlGaAs. By considering the electron–LO–phonon interaction (ELOPI), the energy levels and the wave functions of an electron confined in ASEQWs are obtained. It is found that whether we consider the ELOPI or not, the incident photon frequency ω and parameters U_0 and σ also affect the SHG coefficient obviously.

Key words: Quantum well, second-harmonic generation

1. Introduction

In the past several years, nonlinear optical properties related to intersubband transitions in semiconducting material have aroused much [1–13]. Due to the existence of a quantum confinement effect, nonlinear effects can be enhanced more dramatically in the low-dimension of quantum systems than that in bulk materials. It is also found that nonlinear optical properties have the potential for device application such as high-speed electro-optical modulators and far infrared photodetectors.

Thanks to the fact that the electron–phonon interaction plays an important role in nonlinear optical properties, polaron effects on nonlinear optical properties are discussed by many researchers [14–20]. When we consider the electron–phonon interaction, we find that nonlinear optical properties such as absorption, second-harmonic generation (SHG), and third-harmonic generation in nanostructures are greatly enhanced. The polaron effects of longitudinal optical (LO) phonons is important in the study of low dimensional semiconductor systems. Polaron effects on the linear and nonlinear optical absorption coefficients and refractive index changes in cylindrical quantum dots with applied magnetic field were studied by Wu et al. in 2013 [21]. In 2013, Liu et al. discussed polaron effects on the optical rectification and the SHG in cylindrical quantum dots with a magnetic field [22]. In 2011, Xie presented polaron effects on the optical absorption coefficients and refractive index of an exciton in quantum dots [23]. Xie also discussed polaron effects on the linear and nonlinear optical absorption coefficients and refractive index changes in two-electron quantum dots. From these researches we know that when we consider the electron–phonon interaction, nonlinear optical properties are greatly enhanced. As we all know, the polaron concept was first put forward by Landau [24]. He pointed out that polaron is

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the autolocalized state of a charge carrier in a homogeneous polar medium and originates from the conduction electron or hole together with its self-induced polarization in an ionic crystal or in a polar semiconductor [22].

The purpose of this paper is to study polaron effects on the second harmonic in asymmetrical semiexponential quantum wells. This paper is organized as follows. In section 2, we obtain the eigenfunctions and the energy eigenvalues by solving the Schrödinger equation when we consider polaron effects. We obtain the SHG coefficients by adopting the framework of the compact-density-matrix approach and iterative method. In section 3, we give numerical results and some discussions. In section 4, a brief conclusion is given.

2. Theory

In this paper, we consider an electron confined in asymmetrical semiexponential quantum wells (ASEQWs). When we consider the electron–LO–phonon interaction (ELOPI), the Hamilton of the system, in the effective mass approximation, within the framework of effective mass approximation, can be written as

$$H = H_e + H_{ph} + H_{e-ph}, \tag{1}$$

where

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

is the electron part; here z represents the growth direction of the quantum well, m^* is the effective mass of electron, and $\hbar$ is the Planck constant. U(z) is the parabolic potential, which is given by

$$U(z) = \begin{cases} U_0(e^{z/\sigma} - 1) & z \geq 0 \\ \infty & z < 0, \end{cases} \tag{3}$$

where both U_0 and σ are positive parameters, and

$$H_{ph} = \sum_q \hbar\omega_{LO} a_q^+ a_q, \tag{4}$$

is the phonon part, where a_q^+ and a_q are the creation and annihilation operators for the LO-phonon, and ω_{LO} is the frequency of the optical phonon. H_{e-ph} stands for the Hamiltonian of the ELOPI, which can be written as

$$H_{e-ph} = \sum_q (v_q e^{iq\cdot r} a_q + v_q e^{-iq\cdot r} a_q^+), \tag{5}$$

where

$$v_q = -\frac{i\hbar\omega_{LO}}{q}(\frac{4\pi\alpha_e}{\Omega})^{\frac{1}{2}}(\frac{\hbar}{2m^*\omega_{LO}})^{\frac{1}{4}}, \tag{6}$$

with

$$\alpha_e = \frac{e^2}{2\hbar\omega_{LO}}(\frac{2m^*\omega_{LO}}{\hbar})(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}); \tag{7}$$

here α_e is the electron–phonon coupling constant, ε_0 is the static dielectric constant, ε_∞ is the optical dielectric constant, $\hbar\omega_{LO}$ is the energy of the optical phonon, and Ω is the quantum volume of a quantum well.

The radial eigenfunction Schrödinger equation and the z-direction schrödinger equation in the absence of the ELOPI are expressed as

$$[-\frac{\hbar^2}{2m^*}(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2})+U(z)]\psi_{n,\mathbf{k}}(\mathbf{r})=\varepsilon_{n,\mathbf{k}}\psi_{n,\mathbf{k}}(\mathbf{r}), \tag{8}$$

where $\varepsilon_{n,\mathbf{k}}$ is the energy eigenvalue and $\psi_{n,\mathbf{k}}(\mathbf{r})$ is the eigenfunction. With the method of separation of variables, we can get the eigenfunctions and the energy eigenvalues by

$$\psi_{n,\mathbf{k}}(\mathbf{r})=\psi_n(z)u_c(\mathbf{r})\exp(i\mathbf{k}_{\|}\cdot\mathbf{r}_{\|}), \tag{9}$$

and

$$\varepsilon_{n,\mathbf{k}}=E_n+\frac{\hbar^2}{2m^*}|\mathbf{k}_{\|}|^2, \tag{10}$$

where $u_c(r)$ is the periodic part of the Bloch function in the conduction band at $\mathbf{k}$=0. $\psi_n(z)$ and E_n are the envelope wave function and the energy eigenvalue in the growth direction of ASEQWs, respectively. $\mathbf{k}_{\|}$ and $\mathbf{r}_{\|}$ are the longitudinal wave vector and coordinate in the x-y plane. The Schrödinger equation of the z direction can be expressed as

$$H_z\psi_n(z)=E_n\psi_n(z), \tag{11}$$

here H_z represents the z part of the Hamiltonian H, and it can be given by

$$H_z=-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2}+U(z), \tag{12}$$

In order to reduce the difficulty of the problem, we make the following assumptions:

$$\xi=ae^{\frac{z}{2\sigma}}, a^2=\frac{8m^2U_0\sigma^2}{\hbar^2}, b=\frac{8m^2(U_0+E_n)\sigma^2}{\hbar^2}; \tag{13}$$

thus, Eq. (11) can be rewritten as

$$\xi^2\frac{\mathrm{d}^2\psi_n(\xi)}{\mathrm{d}\xi^2}+\xi\frac{\mathrm{d}\psi_n(\xi)}{\mathrm{d}\xi}-(\nu^2+\xi^2)\psi_n(\xi)=0, \tag{14}$$

here $\nu=i\sqrt{b}$. The above equation is a modified Bessel equation whose solution is [25]

$$\psi_n(\xi)=AK_\nu(\xi)+BI_\nu(\xi), \tag{15}$$

where A and B are arbitrary constants. Because of the fact that $I_\upsilon(\xi)$ increases exponentially when ξ multiplies toward infinity, $I_\upsilon(\xi)$ cannot satisfy boundary conditions, and B must be 0. As a result, Eq. (15) can be rewritten as

$$\psi_n(z)=AK_{i\sqrt{b}}(ae^{\frac{z}{2\sigma}}). \tag{16}$$

We can obtain the normalized coefficient by normalized condition, and the energy eigenvalues E_n can be numerically solved by the standard continuous condition $K_{i\sqrt{b}}(a)=0$ [25].

The eigenfunction of the phonon can be written as $|n\rangle$. Because the ELOPI is rather weak in many materials, we can consider $H_0 = H_e + H_{LO}$ as an unperturbed Hamiltonian and the ELOPI H_{e-ph} as a perturbation. As a result, the unperturbed wave eigenfunction and the eigenvalue have the following form:

$$|\psi_i\rangle = \psi_{n,\mathbf{k}}(\mathbf{r})|n\rangle, \tag{17}$$

$$E_i^0 = \varepsilon_{n,\mathbf{k}} + \sum_q n_q \hbar\omega_{LO}. \tag{18}$$

We limit our consideration to one-phonon absorption. Through the theory of perturbation, the wave function of the system can be expressed as

$$|\Phi_i\rangle = |\psi_i\rangle + \sum_{i\neq j} \frac{\langle \psi_j^0 \mid H_{e-ph} \mid \psi_i^0\rangle}{E_i^0 - E_j^0}|\psi_j\rangle. \tag{19}$$

The energy level of the system with consideration of perturbation is

$$E_i = E_i^0 + \sum_{i\neq j} \frac{|\langle \psi_j^0 \mid H_{e-ph} \mid \psi_i^0\rangle|^2}{E_i^0 - E_j^0}. \tag{20}$$

Next, we will acquire the SHG coefficients by using the compact density matrix method and the iterative procedure. Suppose an electromagnetic field is applied to the system for excitation. The field vector of the applied electromagnetic field is

$$E(t) = E_0 cos(\omega t) = \widetilde{E}\exp(-i\omega t) + \widetilde{E}\exp(i\omega t), \tag{21}$$

where ω is the frequency of the external incident field with a polarization vector normal to the asymmetrical semiexponential quantum wells. It is supposed that ρ is the electronic density matrix of the system. The evolution of ρ obeys the following Liouville's quantum equation:

$$\frac{\partial \rho_{ij}}{\partial t} = \frac{1}{i\hbar}[H_0 - ezE(t), \rho]_{ij} - \Gamma_{ij}(\rho - \rho^{(0)})_{ij}, \tag{22}$$

where Γ_{ij} is the phenomenological relaxation rate, which is caused by the interactions of electron–phonon and electron–electron and other collision processes, $\rho^{(0)}$ is the unperturbed density matrix, H_0 is the Hamiltonian of the system in the absence of the electromagnetic field $\vec{E}(t)$, and ez is the dipole moment operator along the z-axis. For the sake of simplicity, we select $\Gamma_{ij} = \Gamma_1 = 1/T_1$ when $i \neq j$ and $\Gamma_{ij} = \Gamma_2 = 1/T_2$ when $i = j$, where $1/T_1$ and $1/T_2$ are respectively the longitudinal relaxation time and transverse relaxation time of the system. Eq. (22) can be worked out by using the iterative method:

$$\rho(t) = \sum_{n=0}^{\infty} \rho^{(n)}(t), \tag{23}$$

with

$$\frac{\partial \rho_{ij}^{(n+1)}}{\partial t} = \frac{1}{i\hbar}\{[H_0, \rho_{ij}^{(n+1)}] - \Gamma_{ij}\rho_{ij}^{(n+1)}\} - \frac{1}{i\hbar}[ez, \rho^{(0)}]_{ij}E(t). \tag{24}$$

After we expand the electronic polarization, the system of polarization can be expressed as

$$P(t) = \varepsilon_0 \chi_\omega^{(1)} \tilde{E} e^{i\omega t} + \varepsilon_0 \chi_{2\omega}^{(2)} \tilde{E}^2 e^{2i\omega t} + \varepsilon_0 \chi_0^{(2)} \tilde{E}^2 + c.c, \tag{25}$$

where $\chi_\omega^{(1)}$, $\chi_{2\omega}^{(2)}$, and $\chi_0^{(2)}$ are the linear, second-order nonlinear, and optical rectification coefficients, respectively, and ε_0 is the vacuum permittivity. They reflect various optical nonlinear effects. The electronic polarization of the nth order is presented:

$$P^{(n)}(t) = \frac{1}{V} Tr(\rho^{(n)} ez), \tag{26}$$

where V is the volume of interaction and Tr denotes the trace or summation over the diagonal elements of the matrix $\rho^{(n)} ez$.

Finally, by using the compact density matrix approach and the iterative method, the analytical expression of the SHG coefficient in a three-level quantum system is given as follows:

$$\chi_{2\omega}^{(2)} = \frac{\sigma_\upsilon e^3}{\varepsilon_0 \hbar^2} \frac{M_{12} M_{23} M_{31}}{(\omega - \omega_{21} + i\Gamma_0)(2\omega - \omega_{31} + i\Gamma_0)}, \tag{27}$$

where σ_ν is the electron density in the system, $M_{ij} = |\langle \psi_i | z | \psi_j \rangle|$ (i,j=1,2,3) is the off-diagonal matrix element, $\hbar\omega_{21} = E_2 - E_1$, $\hbar\omega_{31} = E_3 - E_1$, Γ_0 is the phenomenological relaxation rate, and $M_{12} M_{23} M_{31}$ is matrix elements' product.

3. Results and discussion

In this section, the above theory is now applied to study polaron effects on SHG in asymmetrical semiexponential quantum wells. We will choose the asymmetry of a quantum well as an example to present the numerical. In the calculations we used the following parameters: $m^* = 0.067 m_0$ (where m_0 is the mass of a free electron), $\sigma_\nu = 5.0 \times 10^{22} m^{-3}$, T_0=0.14ps, $\hbar\omega_{LO}$=36.25 mev, $\varepsilon_0 = 12.83$, $\varepsilon_\infty = 10.9$, and electron–phonon coupling strength α_e= 0.0681.

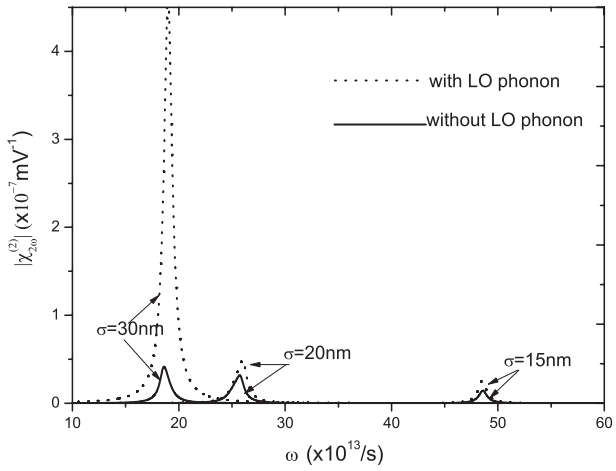

Figure 1. The SHG coefficients $\chi_{2\omega}^2$ as a function of the incident photon frequency ω, with $U_0 = 200$ mev for three different values of the parameter σ, $\sigma = 15$ nm, $\sigma = 20$ nm, $\sigma = 30$ nm.

In Figure 1, the SHG coefficients as function of the incident photon energy with $U_0 = 200$ mev for three different values of σ are shown. The dotted lines and solid lines correspond to two cases: with and without considering the electron-LO-phonon, respectively. From the figure, it can be clearly seen that the SHG coefficients $\chi^{(2)}_{2\omega}$ are enhanced when we consider the ELOPI. The physical reason for the feature is that the wave function of an electron spread to wider space when we consider the ELOPI , which leads to the fact that the overlap of wave function is enhanced. Moreover, we can find a notable feature in the figure, i.e. the peak of SHG coefficients increases with the augment of σ whether we consider the ELOPI. The physical reason for this feature is that the increment of σ makes the overlaps between different electronic states increase, which leads to the increment of matrix elements' product $M_{12}M_{23}M_{31}$. The matrix elements' product $M_{12}M_{23}M_{31}$ is plotted in Figure 2.

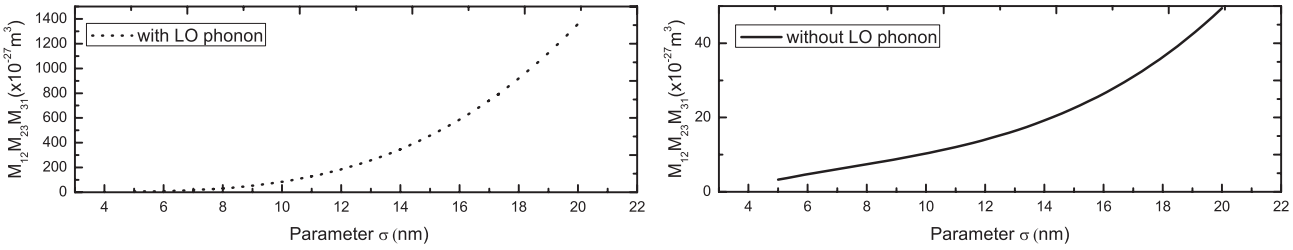

Figure 2. The matrix elements' product $M_{12}M_{23}M_{31}$ as function of σ with $U_0 = 200$ mev.

In Figure 1, we can see that the peaks of the SHG coefficients move toward the lower energy region with the increment of σ. The physical reason for this feature is that the quantum confinement becomes weak with the increment of σ, which leads to a decrease in energy intervals E_{21} and E_{31}. At last ω_{21} and ω_{31} decrease with increasing σ. In Figure 3, we show that the energy intervals decrease with the increment of σ.

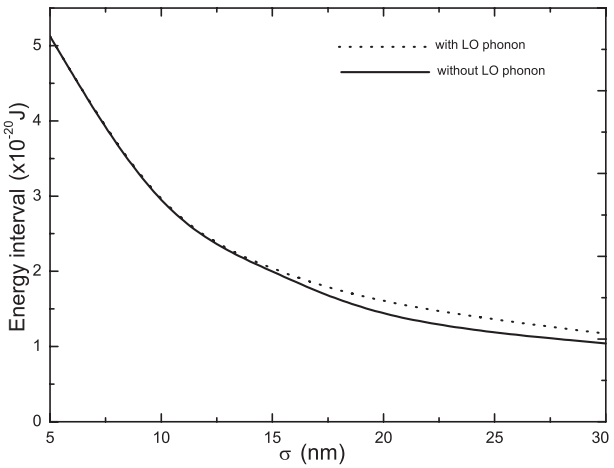

Figure 3. The energy intervals as a function of σ with $U_0 = 200$ mev.

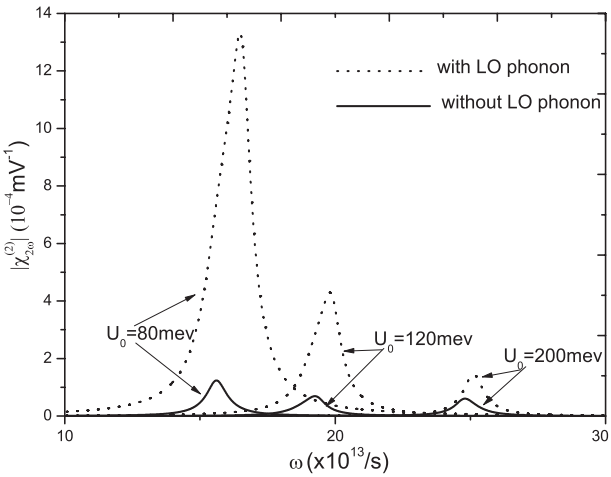

Figure 4. The SHG coefficients $\chi^2_{2\omega}$ as a function of the incident photon frequency ω, with $\sigma = 10$ nm for three different values of the parameter $U_0, U_0 = 80$ mev, $U_0 = 120$ mev, $U_0 = 200$ mev.

In Figure 4, the SHG coefficients as a function of the incident photon energy for three different values of U_0 with $\sigma = 10$ nm are shown. From the figure, it can be clearly seen that when we consider the ELOPI

the SHG coefficient $\chi^{(2)}_{2\omega}$ is enhanced. The physical reason is that the wave function of an electron spread to wider space when we consider the ELOPI, which leads to the fact that the overlap of wave function is enhanced. Moreover, from the figure, it is clearly observed that the resonant peaks of the SHG coefficients decrease with the increment of U_0. The reason for this feature is that whether we take into account ELOPI or not the overlaps between different electronic states become less with the increment of U_0, which leads to a decrease in the matrix elements' product $M_{12}M_{23}M_{31}$. The matrix elements' product $M_{12}M_{23}M_{31}$ is plotted in Figure 5.

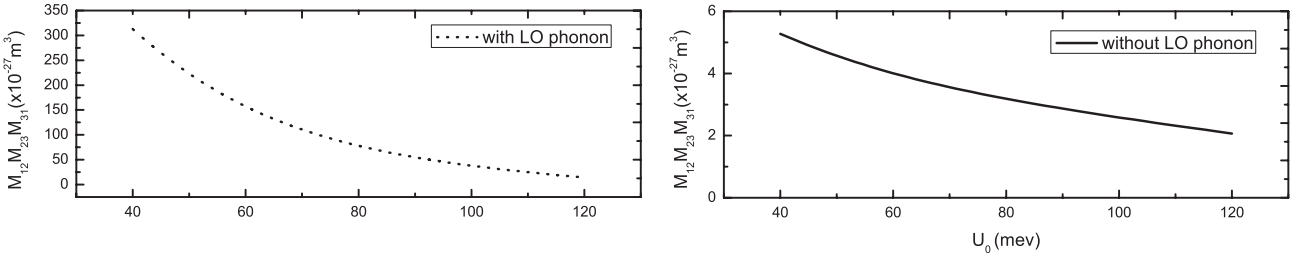

Figure 5. The matrix elements' product $M_{12}M_{23}M_{31}$ as a function of U_0 with $\sigma = 10$ nm.

Furthermore, it is clearly observed that whether the ELOPI is considered or not the resonant peaks of the SHG coefficients $\chi^{(2)}_{2\omega}$ suffer a blue shift. The reason for this characteristic is that whether the ELOPI is considered or not the quantum confinement becomes strong with the increment of U_0, which lead to the increment of E_{21}. ω_{21} increases with the increment of U_0. In Figure 6, we show that energy intervals increase with the increment of U_0. Therefore, the resonant peaks of the SHG coefficients $\chi^{(2)}_{2\omega}$ suffer a blue shift.

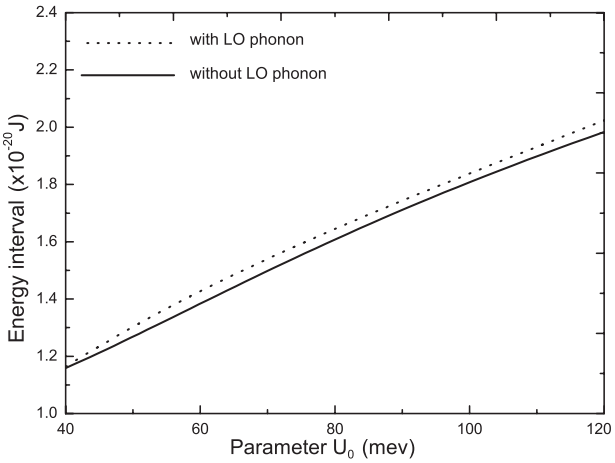

Figure 6. The energy intervals as a function of U_0 with $\sigma = 10$ nm.

4. Conclusion

In this paper, we studied theoretically polaron effects on the SHG and calculations were performed by using the density matrix approach within the effective-mass approximation. The results are presented as a function of incident photon energy. Our calculations mainly focus on the dependence of SHG on photon frequency ω, and parameters σ and U_0. The calculations of our paper reveal that the resonant peak of $\chi^{(2)}_{2\omega}$ is enhanced when the polaron effect is considered. We can also see that whether the polaron effect is consider or not with

the increment of U_0 or the decrement of σ , due to the enhancement of the quantum confinement, a blue shift occurs. Finally, we hope that the results obtained in our research above are valuable theoretically and experimentally for our scientific research in nonlinear optics.

Acknowledgments

This work was supported by the National Natural Science Foundation of China (under Grant No. 61178003, 61475039), Guangdong Provincial Department of Science and Technology (under Grant Nos. 2012A08 0304010, S2012010010115, 2012B091100031, 2012A08 0304005), the Science and Information Technology Bureau of Guangzhou (under Grant No. 11A51020096), and Guandzhou Municipal Department of Education (under Grant No.12A005S).

References

[1] Zhang, L. *Superlatt. Microstruct.* **2005**, *37*, 261–272.

[2] Yu, Y.B.; Zhu, S.N.; Guo, K.X. *Solid State Commun.* **2006**, *139*, 76–79.

[3] Duque, C. M.; Barseghyan, M. G.; Duque, C. A. *Eur. Phy. J. B.* **2010**, *73*, 309–318.

[4] Kasapoglu, E.; Sökmen, I. *Physica E.* **2005**, *27*, 198–203.

[5] Ozturk, E.; Sökmen, I. *Superlatt. Microstruct.* **2010**, *48*, 312–320.

[6] Yesilgul, U.; Sakiroglu, S.; Kasapoglu, E.; Sari, H.; Sökmen, I. *Physica B.* **2011**, *406*, 1441–1444.

[7] Keshavarz, A.; Karimi, M. J. *Phy. Lett. A.* **2010**, *374*, 2675–2680.

[8] Kasapoglu, E.; Sari, H. *Superlatt. Microstruct.* **2001**, *29*, 25–32.

[9] Kasapoglu, E.; Sari, H.; Bursal, M.; Sökmen, I. *Physica E.* **2003**, *16*, 237–243.

[10] Prasad, V.; Silotia, P. *Phys. Lett. A.* **2011**, *375*, 3910–3915.

[11] Yesilgul, U. *J. Lumin.* **2012**, *132*, 765–773.

[12] Ungan, F.; Yesilgul, U.; Sakiroglu, S.; Kasapoglu, E.; Sari, H.; Sökmen, I. *Phy. Lett. A.* **2010**, *374*, 2980–2984.

[13] Kasapoglu, E.; Sari, H.; Sökmen, I. *Solid State Commun.* **2003**, *125*, 429–434.

[14] Li, N.; Guo, K. X.; Shao, S.; Liu, G. H. *Optical Materials* **2012**, *34*, 1459–1463.

[15] Prasad, V.; Silotia, P. *Phys. Lett. A.* **2011**, *375*, 3910–3915.

[16] Yakar, Y.; Cakir, B.; Ozmen, A. *Opt. Commun.***2010**, *283*, 1795–1800.

[17] Xie, W. F. *Optics Communications* **2011**, *284*, 4756–4760.

[18] Kaneko, T.; Koshino, M.; Ando, T. *Phy. Rev. B.* **2008**, *78*, 245303–245311.

[19] Puangmali, T.; Califano, M.; Harrison, P. *Phys. Rev. B.* **2008**, *78*, 245104–245109.

[20] Cho, A. Y.; Arthur, J. R. *Prog. Solid State Chem.* **1975**, *10*, 157–191.

[21] Wu, Q. J.; Guo, K. X.; Liu, G. H. *Physica B.* **2013**, *410*, 206–211.

[22] Liu, G. H.; Guo, K. X.; Wu, Q. J. *Superlatt. Microstruct.* **2013**, *53*, 173–183.

[23] Xie, W. F. *Physica B.* **2011**, *406*, 2858–2861.

[24] Landau, L. D. *Phys. Z. Sowjetunion.* **1933**, *3*, 664–670.

[25] Liu, G. H.; Guo, K. X.; Wu, Q. J. *Superlatt. Microstruct.* **2012**, *52*, 183–192.