INFLUENCE OF THERMALLY INDUCED STRAINS ON THE FORMATION ENERGIES OF 1*s*- AND 2*s*-EXCITONS IN A STRESSED ZnSe/ZnS QUANTUM WELL

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In the framework of the deformation potential model, the formation energies of 1*s*- and 2*s*-excitons in a ZnSe/ZnS quantum well have been calculated taking into account both the mechanical strain appearing in the heterostructure owing to the lattice mismatch between two contacting layers ($f = \Delta a/a \approx 4.5\%$) and the thermally induced strain caused by their different coefficients of thermal expansion ($\Delta\alpha_T/\alpha_T \approx 17\%$). The thermally induced strain component, appearing in the ZnSe/ZnS heterostructure that was grown within the temperature interval 500—700 K and is exploited at 4.2, 77, and 300 K, has been demonstrated to increase the formation energies of 1*s*- and 2*s*-excitons by about 10 meV.

1. Introduction

It is known [1–3] that the recombination of excitons localized in ZnSe/ZnS quantum wells leads to the emission in the blue-green range of the spectrum. Therefore, ZnSe/ZnS-based quantum wells [4, 5] are perspective structures for creating heterolasers in this spectral range.

Internal stresses arise in heterosystems, mainly, owing to a lattice mismatch between two contacting layers, which leads to mismatch stresses; to the different coefficients of thermal expansion of two materials, which results in the appearance of thermally induced strains; and to the presence of defects in heterosystem layers [6]. The first factor and its influence on the ground state energies of 1*s*- and 2*s*-excitons in a ZnSe/ZnS quantum well have been studied in work [7]. There are a relatively small number of heteroepitaxial systems, where the mismatch stress dominates. In particular, those include Ge/GaAs [8], some systems of the $A^{III}B^{V}_{x}C^{V}_{1-x}/A^{III}B^{V}$ type with low x [9], and metal systems with high incommensurability ($\geq 10\%$). In most cases, thermally induced deformations, which emerge in heterostructure layers at the final (cooling) stage of their growing owing to a difference between their thermal factors ($\Delta\alpha_T/\alpha_T \approx 17\%$ [5]) substantially affect the optical and structural properties of heterosystems. Therefore, the variation of a growth temperature modifies the deformation in heterostructure layers (because of its thermally induced component), which, in turn, changes the potential profile of the quantum well; shifts electron, hole, and exciton levels in the heterostructure concerned; i.e. affects the optical properties of heterostructures.

This work aims at calculating the influence of thermally induced strain on the formation energies of 1*s*- and 2*s*-excitons in a ZnSe/ZnS quantum well.

2. Model

Consider a stressed ZnS/ZnSe/ZnS heterosystem with a ZnSe quantum well. If it is cooled from the heterosystem growing temperature ($T_1 = 350 - 700$ K) down to the ambient temperature or even a lower one ($T_2 = 4.2 - 300$ K), the compressive deformation $\varepsilon^i_T(\Delta T)$ emerges in each heterosystem layer (i = ZnSe or ZnS). Owing to a difference between the thermal components of the deformation parameters in contacting materials (because their parameters of thermal expansion α^i_T are not identical), a discontinuity of the thermal deformation appears at the heterointerface [6]:

$$-f_T = \varepsilon^{\mathrm{ZnSe}}_T(\Delta T) - \varepsilon^{\mathrm{ZnS}}_T(\Delta T) =$$

$$= 3\left(\alpha_T^{\mathrm{ZnSe}} - \alpha_T^{\mathrm{ZnS}}\right)(T_2 - T_1.) \quad (1)$$

The deformations are reckoned from a distorted state of the ZnS lattice, resulted from the different coefficients of temperature expansion of the contacting materials. Then, the total deformation in the layers of the ZnSe/ZnS heterostructure is determined by the relations

$$\varepsilon^{\mathrm{ZnS}}(L_w, b) = \varepsilon_f^{\mathrm{ZnS}}(L_w, b). \quad (2)$$

and

$$\varepsilon^{\mathrm{ZnSe}}(L_w, b, \Delta T) =$$

$$= \varepsilon_f^{\mathrm{ZnSe}}(L_w, b) + 3\left(\alpha_T^{\mathrm{ZnSe}} - \alpha_T^{\mathrm{ZnS}}\right)(T_2 - T_1), \quad (3)$$

where $\Delta T = T_1 - T_2$, T_1 is the growth temperature, and T_2 the operation temperature of the heterosystem.

The deformation parameter $\varepsilon_f^i(L_w, b)$ is the function of the lattice parameters $a_{||}(L_w, b)$ (in the plane of the ZnSe/ZnS contact) and $a_\perp^i(L_w, b)$ (perpendicularly to it) [10]:

$$\varepsilon_f^i(L_w, b) = \frac{1}{a^i}\left(2a_\parallel(L_w, b) + a_\perp(L_w, b)\right) - 3, \quad (4)$$

where L_w is the thickness of the ZnSe layer, b the thickness of the ZnS layer, a^i the lattice parameter of the i-th contacting material in bulk,

$$a_\parallel(L_w, b) = \frac{L_w a^{\mathrm{ZnSe}} G^{\mathrm{ZnSe}} + b\, a^{\mathrm{ZnS}} G^{\mathrm{ZnS}}}{L_w G^{\mathrm{ZnSe}} + b G^{\mathrm{ZnS}}}, \quad (5)$$

G^i is the shear modulus of the i-th layer,

$$a_\perp^i(L_w, b) = a^i\left[1 - D_{001}^i\left(\frac{a_\parallel}{a^i} - 1\right)\right] \quad (6)$$

and D^i is defined in terms of elastic constants of the corresponding layer [10].

In order to solve this problem, we use the method of equivalent Hamiltonian [11] which has been developed to find the exciton spectrum in a mechanically stressed ZnSe/ZnS quantum well [7].

We assume the thickness of the ZnSe layer to be small in comparison with the Bohr radius of a Wannier exciton in ZnSe. This enables us to consider the exciton as such that behaves like a two-dimensional hydrogen-like atom in the plane parallel to the layer contact one, and as the electron and the hole, being independent, in the potential well along the heterostructure growth axis. The influence of the finite thickness of the ZnSe layer was calculated making use of perturbation theory.

The spectra of $1s$- and $2s$-excitons in the ZnSe layer were found by solving the Schrödinger equation [7]

$$\left(E_c^{\mathrm{ZnSe}}(\vec{k}) + V_c(z_e) - E_v^{\mathrm{ZnSe}}(\vec{k}) - V_v(z_h) - \right.$$

$$\left. - \frac{e^2}{\varepsilon^{ZnSe}|\vec{r}_e - \vec{r}_h|}\right)\Psi^{\mathrm{ZnSe}}(\vec{r}_e, z_e; \vec{r}_h, z_h) =$$

$$= \left(E - E_{\mathrm{gr}}^{\mathrm{ZnSe}}\right)\Psi^{\mathrm{ZnSe}}(\vec{r}_e, z_e; \vec{r}_h, z_h) \quad (7)$$

where $E_{\mathrm{gr}}^{\mathrm{ZnSe}}$ and $E_{c,v}^{\mathrm{ZnSe}}(\vec{k})$ are the energies of the ground state and the corresponding bands in the ZnSe layer, respectively; c and v are the subscripts that specify the conduction or valence band, respectively;

$$V_c(z_e) = \begin{cases} \Delta E_{0c} + a_c^{\mathrm{ZnS}}\varepsilon^{\mathrm{ZnS}}(L_w, b, \Delta T) - a_c^{\mathrm{ZnSe}}\varepsilon^{\mathrm{ZnSe}}(L_w, b, \Delta T), & |z_e| > \frac{L_w}{2} \\ 0, & |z_e| < \frac{L_w}{2} \end{cases}, \quad (8)$$

$$V_v(z_h) = \begin{cases} \Delta E_{0v} + a_v^{\mathrm{ZnSe}}\varepsilon^{\mathrm{ZnSe}}(L_w, b, \Delta T) - a_v^{\mathrm{ZnS}}\varepsilon^{\mathrm{ZnS}}(L_w, b, \Delta T) + \Delta E_{v,2}^{\mathrm{ZnSe}} - \Delta E_{v,1}^{\mathrm{ZnS}}, & |z_h| > \frac{L_w}{2} \\ 0, & |z_h| < \frac{L_w}{2} \end{cases}, \quad (9)$$

are the potential well energies for an electron and a hole, respectively (Fig. 1,*c*); $\alpha = e, h$; $a_{c,v}^i$ are the constants of the deformation potential in the i-th layer; $\Delta E_{0c,v}$ the discontinuities of the conduction and valence bands, respectively, due to the different chemical structures of the layers; and $E_{v,1}^i$ and $E_{v,2}^i$ denote the bands of light and heavy holes, respectively [5]. These bands are strictly degenerate only provided the absence of uniaxial pressure and spin-orbit splitting. Shear deformations split the top of the valence band at point Γ8, which, together with the spin-orbit effect, governs the ultimate energy positions of the valence bands of light and

heavy holes. These positions are proportional to the strain amplitude, expressed in terms of hydrostatic and uniaxial deformation potentials, and reckoned from the averaged electrostatic potential of the semiconductor $E_{v,\mathrm{av}}$, which is the "center of mass" of the highest valence subbands at point Γ8.

Under the action of a mechanical stress along direction [001] in the heterosystem, the energy positions of the tops of the valence bands of heavy and light holes are determined by the relations [5]

$$\Delta E^i_{v,2} = \tfrac{1}{3}\Delta^i_0 - \tfrac{1}{2}\delta E^i_{001}, \tag{10}$$

$$\Delta E^i_{v,1} = -\tfrac{1}{6}\Delta^i_0 + \tfrac{1}{4}\delta E^i_{001} +$$

$$+\tfrac{1}{2}\left[\left(\Delta^i_0\right)^2 + \Delta^i_0\delta E^i_{001} + \tfrac{9}{4}\left(\delta E^i_{001}\right)^2\right]^{1/2}, \tag{11}$$

$$\Delta E^i_{v,3} = -\tfrac{1}{6}\Delta^i_0 + \tfrac{1}{4}\delta E^i_{001} -$$

$$-\tfrac{1}{2}\left[\left(\Delta^i_0\right)^2 + \Delta^i_0\delta E^i_{001} + \tfrac{9}{4}\left(\delta E^i_{001}\right)^2\right]^{1/2}, \tag{12}$$

where

$$\delta E^i_{001} = 2b^i\left(\varepsilon^i_{zz} - \varepsilon^i_{xx}\right), \tag{13}$$

and b^i is the constant of the shear deformation potential for crystals with tetragonal symmetry.

The potential energy of electrons is reckoned from the bottom of the ZnSe conduction band, and the potential energy of holes from the top of the valence band.

The energy bands in ZnSe are regarded as those in a simple cubic lattice. Taking into account that the rectangular wells $V_c(z_e)$ and $V_v(z_h)$ affect only the motion in the z-direction, expanding the band energies into the series in k_x and k_y up to the terms of the second order, using the effective mass approximation, and substituting the results into Eq. (7), we obtain the Schrödinger equation for the exciton motion in the potential field (8) and (9).

The Hamiltonian of the Schrödinger equation can be decomposed into three components. The first component H_z describes the motion of an electron-hole pair in the quantum well along the direction z:

$$H_z = h_c(z_e) - h_v(z_h), \tag{14}$$

where

$$h_c = \begin{cases} \frac{\hbar^2}{m_e^{*(\mathrm{ZnSe})}(a^{\mathrm{ZnSe}})^2}\left[1-\cos\left(-ia_\perp^{\mathrm{ZnSe}}\frac{\partial}{\partial z_e}\right)\right] + E_0^{\mathrm{ZnSe}}\left(\varepsilon^{\mathrm{ZnSe}}\right) + E_{\mathrm{gap}}^{\mathrm{ZnSe}}\left(\varepsilon^{\mathrm{ZnSe}}\right) + V_c(z_e), & |z_e| < \frac{1}{2}L_w \\ -\frac{\hbar^2}{2m_e^{*(\mathrm{ZnS})}}\frac{\partial^2}{\partial z_e^2} + V_c(z_e), & |z_e| > \frac{1}{2}L_w \end{cases}, \tag{15}$$

$$h_v = \begin{cases} -\frac{\hbar^2}{m_h^{*(\mathrm{ZnSe})}(a^{\mathrm{ZnSe}})^2}\left[1-\cos\left(-ia_\perp^{\mathrm{ZnSe}}\frac{\partial}{\partial z_h}\right)\right] + E_0^{\mathrm{ZnSe}}\left(\varepsilon^{\mathrm{ZnSe}}\right) + V_h(z_h), & |z_h| < \frac{1}{2}L_w \\ \frac{\hbar^2}{2m_h^{*(\mathrm{ZnS})}}\frac{\partial^2}{\partial z_h^2} + V_h(z_h), & |z_h| > \frac{1}{2}L_w \end{cases}, \tag{16}$$

$E_0^{\mathrm{ZnSe}}\left(\varepsilon^{\mathrm{ZnSe}}\right)$ is the energy of the valence band top, and $E_{\mathrm{gap}}^{\mathrm{ZnSe}}\left(\varepsilon^{\mathrm{ZnSe}}\right)$ the energy gap width in ZnSe, renormalized owing to a deformation in the heterostructure layers. The second component H_{xy} describes the coupled motion of an electron and a hole in the plane of the growing layer (the xy plane):

$$H_{xy} = -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial\vec{R}^2_{\mathrm{c.m}}} - \frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial\vec{r}^{\,2}} - \frac{e^2}{\varepsilon r}, \tag{17}$$

where M and μ are the total and the reduced mass of the electron-hole pair, respectively; and $\vec{R}_{\mathrm{c.m.}}$ is the two-dimensional radius vector of the exciton's center of mass. The third component H' describes the perturbation caused by the finiteness of the ZnSe layer thickness:

$$H' = \frac{e^2}{\varepsilon}\left(\frac{1}{r} - \frac{1}{\sqrt{r^2+z^2}}.\right). \tag{18}$$

In this problem, the thickness of the ZnSe layer was taken narrower than the exciton Bohr radius, i.e. $L_w/a_0 < 1$. Provided such an assumption, the component H' of the Hamilton operator can be treated as a perturbation. Then, according to Eqs. (14)—(18), the motions of the electron-hole pair in the xy-plane and along the z-direction are independent. The non-perturbed wave function is taken as a product of the

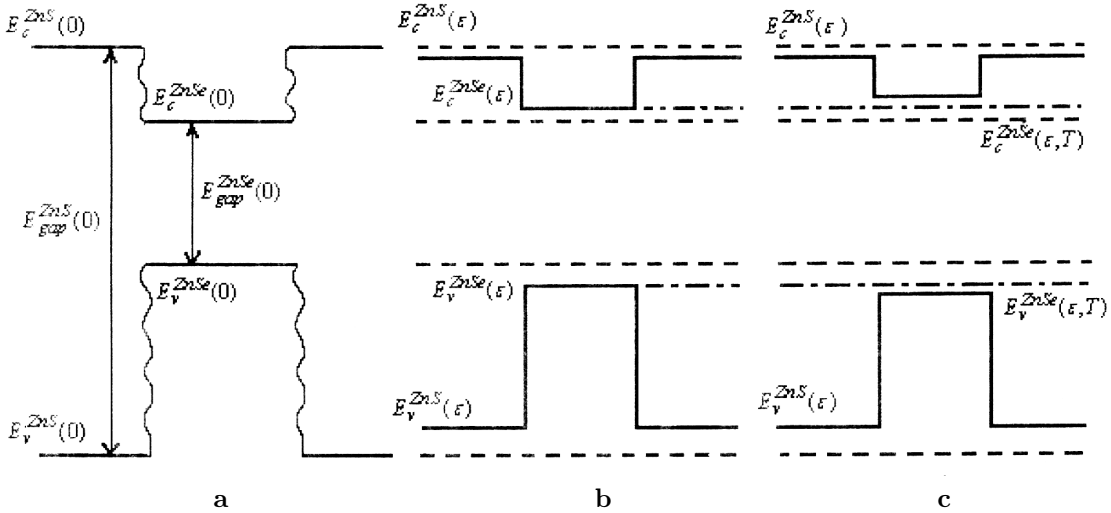

Fig. 1. Energy band schemes for a ZnSe/ZnS quantum well: (a) in a nonstrained ZnSe/ZnS heterostructure, (b) taking a mismatch deformation into account, and (c) taking both thermally induced and mismatch deformations into account

wave functions corresponding to the motion of an electron in the z-direction, the hole's motion in the z-direction, the coupled motion of the electron and the hole in the xy-plane, and the motion of the exciton's center of mass. The corresponding eigenvalues and eigenfunctions are determined from the following equations:

$$h_c\left(z_e\right)\varphi_{k_e}\left(z_e\right) = E_z^{(e)}\varphi_{k_e}\left(z_e\right), \tag{19}$$

$$-h_v\left(z_h\right)\varphi_{k_h}\left(z_h\right) = E_z^{(h)}\varphi_{k_h}\left(z_h\right), \tag{20}$$

$$\left(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial\vec{r}^{\,2}} - \frac{e^2}{\varepsilon r}\right)\psi\left(\vec{r}\,\right) = E_{xy}\psi\left(\vec{r}\,\right), \tag{21}$$

$$-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial\vec{R}_{\rm c.m}^2}\chi\left(\vec{R}_{\rm c.m}\right) = E_R\chi\left(\vec{R}_{\rm c.m}\right), \tag{22}$$

$$\varepsilon^{(0)} = E_z^{(e)} + E_z^{(h)} + E_{xy} + E_R, \tag{23}$$

where the first term in Eq. (23) is the eigenvalue of the electron motion energy in the z-direction, the second term is the same but for the hole, the third term is the energy of the exciton motion in the xy plane, and the fourth term is the motion energy of the exciton's center of mass (for the sake of simplification, it is taken to be zero). The quantity

$$E_{\rm gap}^{\rm ZnSe}(\varepsilon^{\rm ZnSe},T_2) = E_{\rm gap}^{\rm ZnSe}(0,T_2) + a_c^{\rm ZnSe}\varepsilon^{\rm ZnSe}(L_w,b,\Delta T) - a_v^{\rm ZnSe}\varepsilon^{\rm ZnSe}(L_w,b,\Delta T) + \Delta E_{v,2}^{\rm ZnSe} \tag{24}$$

is the energy gap width in ZnSe renormalized owing to the mechanically and thermally induced strains in the heterostructure layers.

3. Numerical Calculations and Discussion of Results

In Fig. 1, the energy band schemes of the ZnSe/ZnS heterostructure are presented, with (panel b) and without (panel c) regard for thermally induced strains. From the scheme in panel c, one can see that the edges of the allowed bands in ZnSe (the bottom of the conduction band and the top of the valence band of heavy holes) shift even more from the relevant positions in non-deformed contacting materials ZnSe/ZnS (panel a), as compared with the case where the deformation is governed by the lattice mismatch only (panel b).

The dependences of the deformation parameter $\varepsilon^{\rm ZnSe}(L_w,b,\Delta T)$ in the ZnSe layer (Eq. (3)) on the difference ΔT between the growth and operation temperatures of the heterostructure are exposed in Fig. 2 for various widths of the quantum well L_w and various barrier thicknesses b. The calculations were carried out for $a^{\rm ZnSe} = 5.65$ Å, $a^{\rm ZnS} = 5.40$ Å, $G_{001}^{\rm ZnSe} = 0.904$ eV/Å^3, $G_{001}^{\rm ZnS} = 1.1269$ eV/Å^3, $D_{001}^{\rm ZnSe} = 1.206$, $D_{001}^{\rm ZnS} = 1.248$ [10], $\Delta E_c(0) = 0.198$ eV, $\Delta E_v(0) = 0.78$ eV, $a_c^{\rm ZnSe} = -3.65$ eV, $a_v^{\rm ZnSe} = 1.75$ eV, $a_c^{\rm ZnS} = -2.78$ eV, $a_v^{\rm ZnS} = 2.31$ eV, $\varepsilon^{\rm ZnSe} = 8.1$, $E_{\rm gap}^{\rm ZnSe}(0) = 2.83$ eV [12], $E_{\rm gap}^{\rm ZnS}(0) = 3.8$ eV, $m_e^{*\rm ZnSe} = 0.17m_0$,

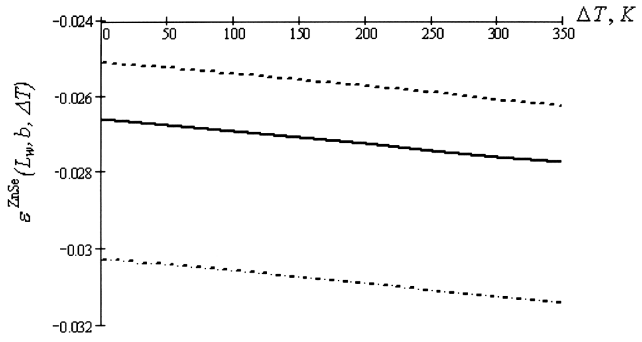

Fig. 2. Dependences of the deformation parameter $\varepsilon^{\mathrm{ZnSe}}(L_w, b, \Delta T)$ in the ZnSe layer of a ZnSe/Zn heterostructure on the difference between the growth and operation temperatures for various thicknesses of the growing layer

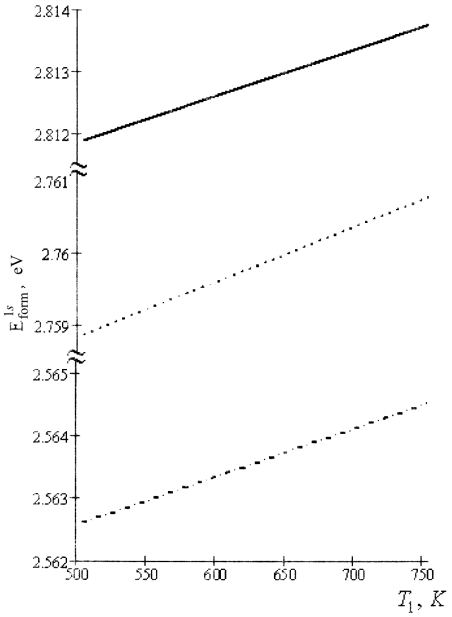

Fig. 3. Dependences of the formation energy of a $1s$-exciton in a ZnSe/ZnS heterostructure on the growth temperature T_1 for various operation temperatures T_2. $b = 50$ Å and $b = 20$ Å

$m_h^{*\mathrm{ZnSe}} = 0.9\ m_0$, $m_e^{*\mathrm{ZnS}} = 0.25 m_0$, $m_h^{*\mathrm{ZnS}} = 0.75\ m_0$[13], $\alpha_T^{\mathrm{ZnSe}} = 7.6 \cdot 10^{-6} K^{-1}$, $\alpha_T^{\mathrm{ZnS}} = 6.5 \times 10^{-6}$ K^{-1} [5], $\Delta_0^{\mathrm{ZnSe}} = 0.43$ eV, $\Delta_0^{\mathrm{ZnS}} = 0.07$ eV, $b^{\mathrm{ZnSe}} = -1.2$ eV, and $b^{\mathrm{ZnS}} = -1.25$ eV [10].

The plots demonstrate that the deformation in the ZnSe layer diminishes monotonously as ΔT grows, which evidences for the emergence of an additional compression. The contribution of the thermally induced deformation to the total deformation in ZnSe equals from 3.5 to 4.2% for the layer thickness values (L_w, b) dealt with in Fig. 2. This contribution decreases as the thickness of the potential barrier b grows and the width of the quantum well L_w decreases, because the mismatch between the lattice constants in the heterojunction plane increases provided such heterostructure parameters, i.e. the contribution of the mismatch deformation parameter $\varepsilon_f^{\mathrm{ZnSe}}(L_w, b)$ grows. Therefore, making allowance for thermally induced stresses in a heterostructure reduces the critical thickness of its layers, at which mismatch dislocations can emerge.

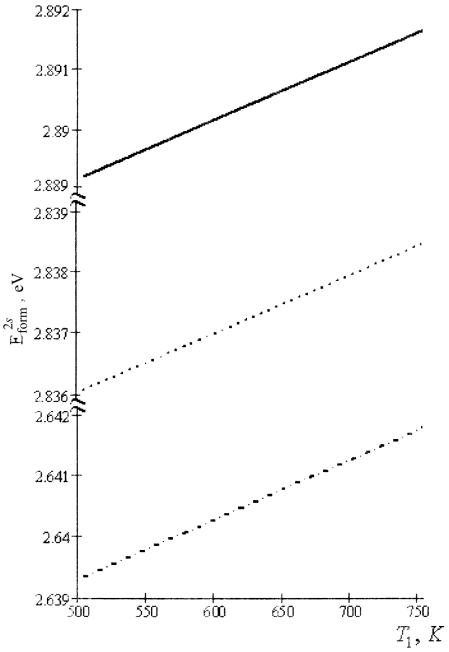

Fig. 4. The same as in Fig. 3, but for a $2s$-exciton

Figs. 3 and 4 depict the results of numerical calculations of the dependences of the formation energies of $1s$- and $2s$-excitons on the heterostructure growth temperature T_1 for various operation ones T_2. One can see that, provided the operation temperature is fixed, the formation energies of $1s$- and $2s$-excitons increase monotonously as the growth temperature rises. Such a behavior of those energies can be explained if we analyze the dependences of their components on the growth temperature:

$$E_{\mathrm{form}}^{1s,2s} = E_z^{(e)} + E_z^{(h)} + E_{\mathrm{gap}}^{\mathrm{ZnSe}}(\varepsilon^{\mathrm{ZnSe}}, T_2) - E_{\mathrm{cpl}}^{1s,2s}, \quad (25)$$

where $E_{\mathrm{cpl}}^{1s,2s} = \left|E_{xy}^{1s,2s}\right| - E'^{1s,2s}$, and $E'^{1s,2s}$ is the correction to the coupling energy, caused by the nonzero ZnSe layer thickness and found in the first approximation of perturbation theory.

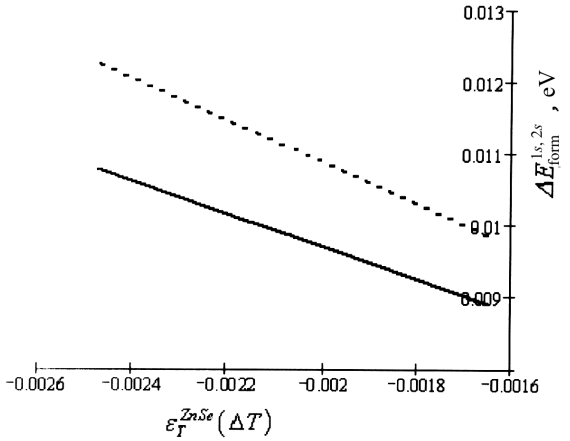

Fig. 5. Variation of the formation energy of a 1s-exciton (solid curve) and a 2s-exciton (dashed curve) in a ZnSe/ZnS heterostructure as the function of the thermally induced strain component in the ZnSe layer at T_1=(500÷750) K and $T_2 = 4.2$ K, $b = 50$ Å, L_w=20 Å

The ground state energies of an electron $E_z^{(e)}$ and a hole $E_z^{(h)}$ grow monotonously as ΔT increases, because the depths of the potential wells for electrons and holes decrease. The greatest contribution to the energy of exciton formation (25) is made by the renormalized, owing to mechanically and thermally induced strains, width of the energy gap in ZnSe $E_{\rm gap}^{\rm ZnSe}(\varepsilon^{\rm ZnSe}, T_2)$, which also grows linearly with T_1. This can be explained by the fact that, as the growth temperature rises, an additional compression in the xy-plane and an additional tension in the direction perpendicular to the layer contact plane (in the z-direction) emerge. This means that the interatomic distances in the ZnSe layer increase in the z-direction, so that the overlapping of wave functions decreases. As a result, the width of the conduction band decreases, and, correspondingly, the width of the energy gap increases.

Therefore, the variation of the formation energies of 1s- and 2s-excitons $\Delta E_{\rm form}^{1s,2s}(L_w, b, \Delta T) = E_{\rm form}^{1s,2s}(L_w, b, \Delta T) - E_{\rm form}^{1s,2s}(L_w, b)$ increase monotonously with the growth of thermally induced strains in the ZnSe layer (Fig. 5). In particular, the increase of the formation energies of 1s- and 2s-excitons, caused by the thermally induced strain component, amounts to 9 and 10 meV, respectively, at $T_1 = 500$ K and $T_2 = 4.2$ K, at to 11 and 12 meV, respectively, at $T_1 = 750$ K and $T_2 = 4.2$ K.

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ВПЛИВ ТЕРМІЧНИХ ДЕФОРМАЦІЙ НА ЕНЕРГІЮ УТВОРЕННЯ 1s- і 2s-ЕКСИТОНІВ У НАПРУЖЕНІЙ КВАНТОВІЙ ЯМІ ZnSe/ZnS

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Р е з ю м е

В рамках моделі деформаційного потенціалу розраховано енергію утворення 1s- і 2s-екситонів у квантовій ямі ZnSe/ZnS з врахуванням як механічної деформації, що виникає в гетеросистемі через неузгодженість параметрів ґраток двох контактуючих шарів ($f = {}^{\Delta a}/_{a} \sim 4,5\%$), так і термічної деформації, спричиненої різними коефіцієнтами термічного розширення (${}^{\Delta\alpha_T}/_{\alpha_T} \approx 17\%$). Показано, що термічна складова деформації ґратки шару ZnSe/ZnS в температурному інтервалі вирощування гетероструктури (500 — 750 K) та при її робочих температурах (4,2, 77 та 300 K) збільшує енергію утворення 1s- та 2s-екситонів приблизно на 10 меВ.