ENERGY SPECTRUM OF ELECTRONS IN A THREE-LAYER HETEROSYSTEM WITH SELF-ORGANIZED DEFECT-DEFORMATION STRUCTURES

R.M. PELESHCHAK, O.V. KUZYK, O.O. DAN'KIV

Ivan Franko Drogobych State Pedagogical University
(24, Ivan Franko Str., Drogobych 82100, Ukraine; e-mail: peleshchak@rambler.ru)

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Equations, which enable the electron energy spectrum in a three-layer heterosystem containing a cluster of point defects in a quantum well to be calculated, have been derived in the framework of the deformation potential method. The dependence of the electron energy difference between the first excited and ground states on the average concentration of point defects of the stretching-center type has been studied for various effective electron masses in a nanocluster material.

1. Introduction

Recently, heterostructures with stressed boundaries or without them have found a wide application in microelectronic devices. Optical and electric properties of semiconductor devices on the basis of quantum wells are known to appreciably depend on the lattice deformation and the spatial distribution of point defects. Such defects can penetrate from the outside or arise in the course of growth. In addition, an important role in the manufacture technology for optoelectronic devices is played by diffusion processes, which are associated with impurities inserted into the semiconductor structure. Extra defects are generated under the influence of external factors, such as heating, deformation, particle bombardment, and others. This influence can be applied purposefully at certain stages of a technological cycle aimed at creating a semiconductor device (irradiation [1, 2], insertion of impurity atoms [3]), or it can be undesirable, for instance, when the device operates under high-radiation conditions.

The interaction between point defects and the self-consistent deformation field, which can arise owing to the very existence of those defects and to the crystal system inhomogeneity (e.g., a heterointerface), gives rise to a spatial redistribution of defects and, under certain conditions, results in the formation of self-organized defect-deformation structures [4–11], such as clusters and periodic structures. In particular, in work [7], a model was developed, which describes the formation of a superlattice composed of antistructural defects emerged under the action of nuclear radiation. Owing to a size mismatch between different atoms, an elastic field emerges around an antistructural defect, so that the defects interact with one another. At a high concentration of antistructural defects, the crystal becomes unstable with respect to a spatially uniform distribution. This instability gives rise to a periodic modulation of the antistructural defect concentration. The interaction of powerful laser pulses with a solid surface is accompanied by the formation of separate clusters and periodic structures, which form a surface relief remaining fixed after the pulse action has terminated [8, 9]. In works [10, 11], the conditions needed for clusters and periodic defect-deformation structures to emerge were found, and the characteristics of those structures – such as their size and shape, the period of periodic structure, and the spatial distributions of deformation and defect concentration – were determined. Calculations were carried out for a bulk material with defect-deformation structures without regard for the electron–deformation interaction.

A non-uniform deformation induced in heterostructures by defect clusters owing to the self-consistent electron–deformation coupling results in a local change of the energy gap width and, accordingly, in a variation of the charge-carrier potential energy. In this work, the regularities in the reconstruction of localized electron levels in three-layer heterosystems under the influence of a deformation induced by the presence of a point-defect cluster in a quantum well are established.

2. Model

In works [4, 5], we showed that the defect-deformation structures can be formed in planar heterostructures with point defects, the average concentration N_{d0} of which exceeds some critical value. In particular, in the defect concentration range $N_{dc1} < N_{d0} < N_{dc}$, there emerges a

one-dimensional cluster, in a vicinity of which the defect distribution along the heterostructure layers and, hence, the lattice deformation are considered to be uniform, whereas, in the direction perpendicular to heterostructure layers, the deformation $U(x)$ is described by the formulas [4, 5]

$$U(x) = \mathrm{sign}\theta_d \frac{A}{B + \mathrm{sh}(-\sqrt{a}x)}, \quad N_{dc1} < N_{d0} < N_{dc2}, \tag{1}$$

$$U(x) = \mathrm{sign}\theta_d \frac{A}{B + \mathrm{ch}(\sqrt{a}x)}, \quad N_{dc2} < N_{d0} < N_{dc}, \tag{2}$$

where (see work [10])

$$N_{dc} = \frac{\rho c_l^2 kT}{\theta_d^2}; N_{dc1} = N_{dc}\left(\frac{l_0}{l_d}\right)^2;$$

$$N_{dc2} = N_{dc}\left(1 - \frac{2\alpha^2}{9\beta}\right); \quad \frac{2\alpha^2}{9\beta} = \frac{4}{9};$$

$$A = 3\sqrt{2}\,|a|\left(\left|9ca - 2f^2\right|\right)^{-1/2};$$

$$B = \sqrt{2}f\left(\left|9ca - 2f^2\right|\right)^{-1/2};$$

$$a = \frac{1 - \frac{N_{d0}}{N_{dc}}}{l_d^2\frac{N_{d0}}{N_{dc}} - l_0^2}; \quad f = \frac{|\alpha|}{l_d^2\frac{N_{d0}}{N_{dc}} - l_0^2}; \quad c = \frac{\beta}{l_d^2\frac{N_{d0}}{N_{dc}} - l_0^2};$$

ρ is the medium density; c_l the longitudinal sound velocity; $\theta_d = K_A\Delta\Omega$ the deformation potential; $\Delta\Omega$ the change of the crystal volume induced by one defect; K_A the bulk elastic modulus; l_d and l_0 are the characteristic lengths of the interaction of defects with crystal atoms and atoms with one another, respectively; α and β are the constants of elastic anharmonicity; T is the temperature; and k the Boltzmann constant.

If the defect concentration in the semiconductor material is low, $N_{d0} < N_{dc1}$, nonlinear effects are insignificant, and the process of self-organization of defects does not occur. In the intervals of the point defect concentration $N_{dc1} < N_{d0} < N_{dc2}$ and $N_{dc2} < N_{d0} < N_{dc}$, the role of a nonlinear interaction between defects by means of the elastic deformation field grows, and, as a result, either an antisymmetric (formula (1)) or symmetric (formula (2)) cluster is formed. At a medium defect concentration in the heterosystem, $N_{d0} > N_{dc}$, periodic defect-deformation structures are formed [5]. The specific values of critical concentrations N_{dc1}, N_{dc2}, and N_{dc} are governed by the elastic constants of the material, the variation of the crystal volume per one defect, and the temperature. At room temperature, the critical concentrations for semiconductors (GaAs, InAs, CdTe, ZnTe) fall within the intervals $N_{dc1} = 10^{17} \div 10^{21}$ cm^{-3}, $N_{dc2} = 5 \times 10^{17} \div 5 \times 10^{21}$ cm^{-3}, and $N_{dc} = 10^{18} \div 10^{22}$ cm^{-3}, the specific values depending on the defect type – the interstitial atom, the vacancy, or the substitutional impurity.

A non-uniform deformation that arises in a vicinity of the cluster shifts the conduction band bottom by $\Delta W(x) = a_c U(x)$, where $a_c < 0$ is the constant of the hydrostatic deformation potential of the conduction band.

Let us consider a three-layer heterostructure (e.g., GaAs/InAs/GaAs), which contains a defect cluster in the quantum well. The potential energy of an electron in this structure is described by the relation

$$W(x) = \begin{cases} \Delta E_c, & |x| \geq b, \\ a_c U(x), & |x| \leq b, \end{cases} \tag{3}$$

where ΔE is a mismatch between the conduction bands of the contacting materials in the heterosystem, and $2b$ is the quantum well width (the width of the InAs interlayer).

Figure 1 schematically illustrates the coordinate dependences of the electron potential energy (solid curves) in the three-layer heterostructure with a nanocluster of point defects of the stretching- ($\theta_d > 0$, panel a) and squeezing-center ($\theta_d < 0$, panel b) types, as well as their approximations by rectangular potentials (dotted curves). The energy is reckoned from the bottom of the conduction band in a nondeformed material, of which the heterostructure interlayer is made. The electron–deformation interaction distorts the potential well, and the latter acquires a complicated shape with an additional dip (barrier) induced by the point defect cluster, in a vicinity of which a non-uniform tensile (compressive) deformation arises.

For the description to be more rigorous, let us replace the electron potential energy in a vicinity of the cluster by a rectangular potential, provided that the numbers of defects in the real and model potential wells are identical [12]. Potential (3) can be approximated by the function

$$W(x) = \begin{cases} \Delta E_c, & |x| \geq b, \\ 0, & d \leq |x| \leq b, \\ -W_0, & |x| \leq d, \end{cases}, \tag{4}$$

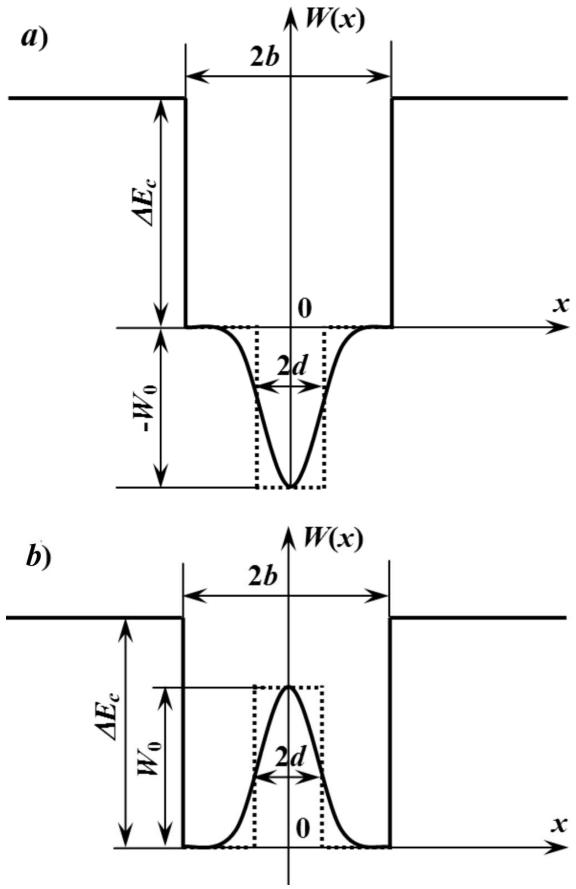

Fig. 1. Coordinate dependences of the electron potential energy in a heterosystem with a defect cluster at $\theta_d > 0$ (a) and $\theta_d < 0$ (b)

where $W_0(N_{d0}) = \mathrm{sign}\theta_d \frac{|a_c|A(N_{d0})}{B(N_{d0})+1}$ is the energy depth of an additional well (the height of an additional barrier), which coincides with the maximum depth of the real potential well (the height of the real potential barrier), and $2d(N_{d0})$ is the additional well (additional barrier) width, which is determined from the condition of the equal numbers of defects in the real and model potential wells.

Taking Eq. (2) into account and bearing in mind that, in the linear approximation, the defect concentration can be written down in the form $N_d(x) \approx \frac{K_A}{\theta_d} U(x)$ [4], the width of the additional potential well can be determined from the condition

$$\int_{-b}^{b} U(x)dx = 2d\,U(0) = \frac{2d\,A}{B+1}, \tag{5}$$

where $U(0)$ is a deformation at the cluster center.

The case illustrated in Fig. 1,b can be realized only provided that the defect concentration is substantial (of about 10^{22} cm^{-3}). This circumstance is related to the fact that the deformation potential θ_d for squeezing-center defects (vacancies, substitutional impurities with the ionic radius shorter than that of matrix atoms) is much lower than the deformation potential of interstitial atoms, which are stretching centers [13]. Accordingly, the critical concentration N_{dc2}, at which the formation of clusters becomes possible, is much higher than that in the case of stretching-center defects. Therefore, in what follows, we confine the consideration to the first case (Fig. 1,a), which corresponds to the existence of a stretching-center defect cluster in the quantum well. The potential well with such a profile is used in resonant-tunneling diodes [14, 15]. In works [14, 15], it was shown that the current-voltage characteristics of such a resonant-tunneling diode are more contrast, i.e. the ratio between the maximum and minimum current values is higher, than the corresponding characteristics of a resonant-tunneling diode with a simple well.

The energy E and the wave function ψ of an electron in the examined system were found by solving the Schrödinger equation

$$\hat{H}\psi = E\psi \tag{6}$$

with the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m_i}\Delta + W, \tag{7}$$

where m_i is the effective mass of the electron in the external layers of heterostructure ($i = 1$) and in the wide ($i = 2$) and narrow ($i = 3$) wells. Since the potential is invariant with respect to the inversion $W(-x) = W(x)$, the solutions of Eq. (6) must be either even or odd.

Even solutions, for which $\psi(-x) = \psi(x)$, can be written down in the interval $x \geqslant 0$ in the form

$$\psi_1(x) = A_1 e^{-k_1(x-b)}, \quad x \geq b, \tag{8}$$

$$\psi_2(x) = A_2 \cos(k_2 x) + A_3 \sin(k_2 x), \quad d \leq x \leq b, \tag{9}$$

$$\psi_3(x) = A_4 \cos k_3 x, \quad 0 \leq x \leq d, \tag{10}$$

where $k_1 = \sqrt{\frac{2m_1(\Delta E_c - E)}{\hbar^2}}$, $k_2 = \sqrt{\frac{2m_2 E}{\hbar^2}}$, $k_3 = \sqrt{\frac{2m_3(W_0+E)}{\hbar^2}}$, and A_1, A_2, A_3, and A_4 are constants. Solution (8) provides the wave function finiteness as $x \to \infty$. In addition, the continuity conditions must be obeyed for the wave function and the probability flow

density at the points $x = b$ and $x = d$,

$$\begin{cases} \psi_1(b) = \psi_2(b), \\ \dfrac{1}{m_1}\dfrac{d\psi_1}{dx}\Big|_{x=b} = \dfrac{1}{m_2}\dfrac{d\psi_2}{dx}\Big|_{x=b}, \\ \psi_2(d) = \psi_3(d), \\ \dfrac{1}{m_2}\dfrac{d\psi_2}{dx}\Big|_{x=d} = \dfrac{1}{m_3}\dfrac{d\psi_3}{dx}\Big|_{x=d}. \end{cases} \tag{11}$$

System of equations (11) has a nontrivial solution at $E > 0$, provided that

$$\mathrm{tg}\,(k_2(b-d)) - \frac{m_2 k_1}{m_1 k_2} + \frac{m_2 k_3}{m_3 k_2}\mathrm{tg}\,(k_3 d) + \\ + \frac{m_2^2 k_1 k_3}{m_1 m_3 k_2^2}\mathrm{tg}\,(k_3 d)\,\mathrm{tg}\,(k_2(b-d)) = 0, \tag{12}$$

and at $E < 0$, if

$$-\mathrm{th}\,(k_2(b-d)) - \frac{m_2 k_1}{m_1 k_2} + \frac{m_2 k_3}{m_3 k_2}\mathrm{tg}\,(k_3 d) + \\ + \frac{m_2^2 k_1 k_3}{m_1 m_3 k_2^2}\mathrm{tg}\,(k_3 d)\,\mathrm{th}\,(k_2(b-d)) = 0. \tag{13}$$

Those conditions can be used to determine the electron ground-state energy, which depends on the defect concentration and the elastic constants of a material.

Odd solutions, for which $\psi(-x) = -\psi(x)$, can be written down in the interval $x \geqslant 0$ in the form

$$\psi_1(x) = B_1 e^{-k_1(x-b)}, \quad x \geq b, \tag{14}$$

$$\psi_2(x) = B_2\cos(k_2 x) + B_3\sin(k_2 x), \quad d \leq x \leq b, \tag{15}$$

$$\psi_3(x) = B_4\sin k_3 x, \quad 0 \leq x \leq d, \tag{16}$$

where B_1, B_2, B_3, and B_4 are constants. In this case, the system of equations (11) has a nontrivial solution at $E > 0$ if

$$\mathrm{tg}\,(k_2(b-d)) + \frac{m_1 k_2}{m_2 k_1} + \frac{m_3 k_2}{m_2 k_3}\mathrm{tg}\,(k_3 d) - \\ - \frac{m_1 m_3 k_2^2}{m_2^2 k_1 k_3}\mathrm{tg}\,(k_3 d)\,\mathrm{tg}\,(k_2(b-d)) = 0, \tag{17}$$

and at $E < 0$ if

$$\mathrm{th}\,(k_2(b-d)) + \frac{m_1 k_2}{m_2 k_1} + \frac{m_3 k_2}{m_2 k_3}\mathrm{tg}\,(k_3 d) + \\ + \frac{m_1 m_3 k_2^2}{m_2^2 k_1 k_3}\mathrm{tg}\,(k_3 d)\,\mathrm{th}\,(k_2(b-d)) = 0. \tag{18}$$

From those conditions, one can determine the energy of an electron in the first excited state.

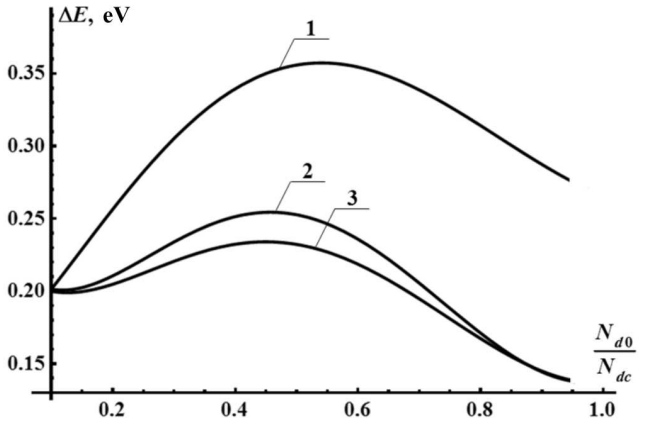

Fig. 2. Dependences of the electron energy difference ΔE between the first excited and ground states in a GaAs/InAs/GaAs heterostructure with a defect nanocluster in the InAs quantum well on the average defect concentration at $m_3/m_0 = 0.03$ (*1*), 0.07 (*2*), and 0.09 (*3*)

3. Calculation Results and Their Discussion

We used relations (12), (13), (17), and (18) to calculate the electron energy in the ground, E, and first excited, E_1, states, as well as the difference between them, $\Delta E = E_1 - E_0$. The latter parameter is important for CVCs of resonant-tunneling diodes [15]. Namely, the quantity ΔE determines the current magnitude at the CVC minimum. The increase of ΔE leads to a reduction of the minimum current magnitude and, accordingly, to the growth of the CVC contrast for resonant-tunneling structures. The calculations were carried out for the GaAs/InAs/GaAs heterosystem characterized by the following parameters: $\Delta E_c = 0.83$ eV, $a_c = -5.08$ eV, $m_1 = 0.065m_0$, $m_2 = 0.057m_0$, $b = 4$ nm, $l_0 = 0.5$ nm, $l_d = 1.6$ nm, $\alpha = 31.88$, and $\frac{2\alpha^2}{9\beta} = \frac{4}{9}$ [10].

In Fig. 2, the dependences of the energy difference for an electron in the first excited and ground states, ΔE, in a GaAs/InAs/GaAs heterostructure with a nanocluster in the InAs quantum well on the average defect concentration are shown for various values of effective electron mass in the cluster material, m_3. The dependences have a nonmonotonous character with a maximum in a vicinity of the point $N_{d0} \approx 0.5N_{dc}$. At the point-defect concentration $N_{d0} \sim 0.1N_{dc}$ (for the InAs semiconductor with interstitial In, $N_{dc} \approx 10^{19}$ cm^{-3}), the cluster is small ($d \to 0$), and ΔE is equal to the corresponding value for a heterostructure free of a defect cluster, which amounts to 0.2 eV at the given parameter values. If the defect concentration increases to $N_{d0} \approx 0.56N_{dc}$ (Fig. 2, curve *1*), the nanocluster size and, respectively, the width of the additional potential well for electrons

grow, which results in that the ground-state energy decreases, whereas the energy of the first excited state increases, so that their difference ΔE becomes larger. The further growth of the defect concentration makes the cluster bigger, but the depth W_0 of the additional potential well, which arises owing to the presence of a nanocluster, decreases, and, at $N_{d0} \to N_{dc}$, the potential well depth tends to zero ($W_0 \to 0$). As a result, the energies of the electron in the ground and first excited states increase. However, the increment in the first excited state is insignificant, so that the value of ΔE diminishes.

As is seen, the presence of a cluster of defects of the stretching-center type increases ΔE by 80% at $N_{d0} = 0.56N_{dc}$, that should find its reflection in the CVCs of resonant-tunneling diodes as a reduction of the minimum current value.

The change of the energy difference for the electron in the first excited and ground states depends substantially on the effective electron mass (Fig. 2). Namely, the increase of ΔE is considerable only if the effective mass of the electron in a nanocluster material is small. In the case where the effective mass of the electron in the nanocluster material is larger than that in the material of the main well (InAs), the growth of ΔE is insignificant, and, at $N_{d0} > 0.7N_{dc}$, this difference is less than the corresponding value for the structure concerned without a defect cluster. This effect can be explained by the fact that the change of the electron energy in the examined structure is governed by two factors: (i) the change of the electron potential energy invoked by deformation effects owing to the presence of the cluster and (ii) the change of the kinetic energy due to the difference between the relevant effective masses. In the former case (the effective mass of the electron in the nanocluster material is smaller than the corresponding value in the main well), both factors act to increase ΔE. In the opposite case (the effective mass of the electron in the nanocluster material is larger than the corresponding value in the main well), they compete with each other; namely, the growth of the effective mass gives rise to a reduction of the electron energy difference ΔE between the first excited and ground states.

4. Conclusions

1. The presence of a nanocluster composed of point defects of the stretching-center type in the interlayer of a three-layer heterostructure results in the formation of an additional potential well (or a potential barrier, if the defects are of the squeezing-center type).

2. We have derived the equations, which allow the energy spectrum of electron in a three-layer heterostructure containing a cluster of point defects in a quantum well to be calculated.

3. The dependence of the difference between the electron energies in the first excited and ground states on the average point defect concentration is studied for various values of effective electron mass in the nanocluster material. The examined difference was shown to be larger than the corresponding value in the structure free of the defect cluster, if the effective mass of the electron in the nanocluster is less than that in the quantum well.

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ЕНЕРГЕТИЧНИЙ СПЕКТР
ЕЛЕКТРОНІВ У ТРИШАРОВІЙ
ГЕТЕРОСИСТЕМІ ІЗ САМООРГАНІЗОВАНИМИ
ДЕФЕКТНО-ДЕФОРМАЦІЙНИМИ СТРУКТУРАМИ

Р.М. Пелещак, О.В. Кузик, О.О. Даньків

Р е з ю м е

У межах методу деформаційного потенціалу отримано рівняння, які дозволяють розрахувати енергетичний спектр електрона у тришаровій гетеросистемі, що містить кластер точкових дефектів у квантовій ямі. Досліджено залежність різниці енергій електрона в першому збудженому та основному станах від середньої концентрації точкових дефектів виду центра розтягу при різних значеннях ефективної маси електрона в матеріалі нанокластера.