ELECTRONIC TRANSITIONS IN QUANTUM DOTS InAs/GaAs WITH HYDROGEN

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Introduction

Recently new method of management of optical properties of heterostructures with quantum dots has been developed intensively – it is introduction in the quantum dot (QD) of an impurity, in particular, of atomic hydrogen. The technology of introduction of atomic hydrogen in the quantum dot is founded on presence of a stream of atomic hydrogen during growth heterosystem with quantum dots by a method of a molecular-beam epitaxy (MBE) [1]. This problem is of interest as for a modern optoelectronics, heliumenergetics, and for one-electron devices, which can find application in the quantum computer [2]. The atomic hydrogen in the quantum dot fulfills two basic functions: it passivates electrically active centres in QD, if they are present [3], and changes the width of quantum dot optical gap owing to change of volume of material of the quantum dot caused by the mismatch between the size of the region of its implantation and radius of hydrogen atom (~ 0,50 Å).

The purpose of this work is the calculation of energy of the basic optical transition in QD with an atomic hydrogen within the framework of model of deformation potential and ascertaining of dependence of shift of this energy on the QD dimension.

The Model

In this problem the InAs quantum dots of spherical symmetry (R_0) disposed in a GaAs semiconductor matrix in radius R_1 are considered. At centre of a QD there is an ionized atom of hydrogen. To reduce a problem with plenty of QD to a problem with a single QD, the following approximation is adopted: the energy of pair-wise elastic interaction between QD is replaced by the energy of interaction of every QD with a mean field of elastic deformation $\sigma_{ef}(N-1)$ of all other QD.

We represent spherical quantum dot of radius R_0 with the ionized atom of hydrogen as a elastic dilatation microinclusion as an elastic ball, inserted into a spherical cavity in a GaAs matrix, the volume of the cavity being smaller than that of the microinclusion by ΔV. For such a spherical microinclusion to be inserted into the matrix, the former must be squeezed, while the surrounding GaAs matrix to be stretched, both in radial directions. The result of simultaneous actions of deformations of contacting nanomaterials is described by the variation of volume ΔV expressed in terms of the parameter $f(R_0, R_1)$:

$$\Delta V(R_0, R_1) = f(R_0, R_1)\cdot 4\pi R_0^3 . \qquad (1)$$

where

$$f(R_0, R_1) = f_1(R_0, R_1) + f_2(R_0, R_1), \qquad (2)$$

where $f_1(R_0, R_1)$, $f_2(R_0, R_1)$ are the relative variations of the lattice parameters of the QD and the surrounding matrix materials, respectively, caused by difference between the radial, $a_r^{(i)}$, and angular, $a_\theta^{(i)}$, $a_\varphi^{(i)}$, components of the lattice parameters both in the QD and the surrounding matrix materials, with respect to their values a_i in unstrained bulk InAs and GaAs materials

$$f_i(R_0, R_1) = \frac{1}{3a_i}\left(2a_\theta + a_r^{(i)}\right) - 1 , \qquad (3)$$

$$a_\theta = a_\varphi = \frac{a_1 G_1 R_0 + a_2 G_2 (R_1 - R_0)}{G_1 R_0 + G_2 (R_1 - R_0)};$$

$$a_r^{(i)} = a_i\left(1 - D_{001}^{(i)}\cdot\left(\frac{a_\theta}{a_i} - 1\right)\right); \qquad D_{001}^{(i)} = 2\frac{C_{12}^{(i)}}{C_{11}^{(i)}};$$

$C_{11}^{(i)}$, $C_{12}^{(i)}$ are the elastic constants of InAs (i = 1) and GaAs (i = 2) materials;
G_1; G_2 are the shear moduluses of materials InAs and GaAs.

Sinse $\dfrac{R_1}{R_0} >> 1$, then $\dfrac{f_2}{f_1} << 1$.

Mechanical stress $\sigma_{rr}^{(i)}$ in InAs and GaAs materials is equal:

$$\sigma_{rr}^{(i)} = \frac{E_i}{(1+\nu_i)(1-2\nu_i)}\left[(1+\nu_i)\varepsilon_{rr}^{(i)} + \nu_i\left(\varepsilon_{\varphi\varphi}^{(i)} + \varepsilon_{\theta\theta}^{(i)}\right)\right],$$

where ν_i, E_i are Poisson's ratios and Young's moduli of the QD and the surrounding matrix materials, which are expressed in the known way in terms of the elastic constants of these materials.

To define the components of the strain tensor $\varepsilon_{lk}^{(i)}$, it is necessary to find explicit forms of atom displacements $u_r^{(1)}$, $u_r^{(2)}$ in InAs and GaAs materials, respectively. With this purpose in view, we write down the equations of balance:

$$\vec{\nabla}\mathrm{div}\vec{u}_i = -D_i \cdot \vec{F}^{(i)}(\vec{r}) \qquad (4)$$

with the boundary conditions for a spherical QD:

$$\begin{cases} 4\pi R_0^2 \left(u_r^{(2)}\big|_{r=R_0} - u_r^{(1)}\big|_{r=R_0} \right) = \Delta V, \\ \sigma_{rr}^{(1)}\big|_{r=R_0} = \sigma_{rr}^{(2)}\big|_{r=R_0} + P_L, \\ \sigma_{rr}^{(2)}\big|_{r=R_1} = -\sigma_{ef}(N-1); \end{cases} \qquad (5)$$

(The left hand side of the first equations of system (5) is equal to a geometrical odds ΔV of the microinclusion and the cavity volumes in the GaAs matrix). Here:

$$D_i = \frac{(1+\nu_i)(1-2\nu_i)}{E_i(1-\nu_i)};$$

$$\vec{F}^{(i)} = \frac{2\Delta\Omega}{3\pi^{3/2}}\left(C_{11}^{(i)} + C_{12}^{(i)}\right)\frac{1}{r_0^5} r e^{-\frac{r^2}{r_0^2}} \frac{\vec{r}}{|\vec{r}|}$$

is volumetric force created by an impurity of hydrogen in a QD; $\Delta\Omega$ is the variation of volume of the QD material, caused by presence of an impurity of hydrogen; r_0 is effective radius of hydrogen atom; $P_L = \frac{2\alpha\left(\varepsilon^{(1)}\right)}{R_0}$ is the Laplace pressure, $\alpha\left(\varepsilon^{(1)}\right)$ is the QD (InAs) surface energy, which is the function of the QD surface stress, $\sigma_{ij}^{(1)}$, and deformation, $\varepsilon_{ij}^{(1)}$, tensors:

$$\begin{aligned} \alpha\left(\varepsilon^{(1)}\right) &= \alpha(0) + \sum_{i,j} \sigma_{ij}^{(1)}\varepsilon_{ij}^{(1)} + \\ &+ \frac{1}{2}\sum_{i,j,k,l} \varepsilon_{ij}^{(1)}(1) \cdot s_{ijkl}^{(1)} \cdot \varepsilon_{kl}^{(1)} + \ldots, \end{aligned} \qquad (6)$$

where $s_{ijkl}^{(1)}$ is the stress tensor of the second order.

Results and discussion

The energy of transition into the ground state in a stressed QD is defined:

$$\begin{aligned} E(\varepsilon) &= E_g^{(2)} - \left|a_c^{(2)} \cdot \varepsilon^{(2)}(R_0, R_1)\right| - \\ &- \left|a_\upsilon^{(2)} \cdot \varepsilon^{(2)}(R_0, R_1)\right| - \left|E_0^{(e)}\right| - \left|E_0^{(h)}\right|, \end{aligned} \qquad (7)$$

where $E_0^{(e,h)}$ is the ground state energy of electron and hole in a stressed QD, digitized from a level of vertex of a potential hill; $a_c^{(2)}$, $a_\upsilon^{(2)}$ are the constants of the hydrostatic deformation potential of the conduction and valence bands, respectively, in GaAs material.

It is possible to explain the dependence of variation of energy width of the basic optical transition ($E = E^0 + \Delta E_\varphi + \Delta E_{def}$) in a coherent-strain QD with an ionized atom of hydrogen on its size R_0 by different behaviour of competing components ΔE_φ and ΔE_{def} with magnification R_0 (E^0 is a component corresponding to energy of the basic optical transition in a pure undeformed QD; ΔE_φ is a component of transition energy caused by presence of the ionized atom of hydrogen; ΔE_{def} is a component of transition energy caused by deformation potential in a pure QD).

With magnification of the size R_0 of the quantum dot both with an impurity of hydrogen and without it, the energy of the basic optical transition decreases monotonically, so that the optical transition moves to long-wave area. At smaller radii ($R_0 \sim 40Å \div 57Å$) the energy width of the basic optical transition E in quantum dots with impurities of hydrogen is larger than unblended, and at larger ones ($R_0 \geq 58Å$) the reverse effect is observed.

Conclusions

It is ascertained that in quantum dots of smaller size (R_0 = 40 Å ÷ 58 Å) the impurity of hydrogen increases the width of the QD optical gap (on 220meV at R_0 = 40 Å), and in QD of larger size $R_0 \geq$ 58 Å it decreases the size of the QD optical gap. Moreover, with increasing of the size of the QD in a range 40 Å $\leq R_0 \leq$ 58 Å the influence of hydrogen impurity on the width of an optical gap decreases and at R_0 = 58 Å absent, since the compensation of action of hydrogen impurity of deformation potential of the QD occurs.

References

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