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Band Structure Modifications of Deformed InP Quantum Wires

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The work describes the features of the band structure of deformed InP nanowires with different diameters. It is shown that the bending of quantum wires is capable of creating local minima in the conduction and valence bands which are separated from the surface of the cylindrical wire. This result opens up new possibilities for controlling both the lifetime of photoexcited carriers by keeping them at these minima and the magnitude of the photovoltage in solar energy conversion devices based on quantum wires. The work lies within a common goal aiming to develop new methods of functionalization of nanostructured surfaces using mechanical deformations.

Keywords: Quantum wire, Mechanical deformation, Charge carriers.

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1. INTRODUCTION

The rapid progress achieved in the synthesis of nanowires by the VLS (vapor-liquid-solid) method [1] has allowed to create semiconductor quantum wires of the diameter to 3 nm [2] (less than ten atoms along the wire diameter) as well as the realization of conducting channels of the field-effect transistors of the length to 40 nm [3]. Evolution of the physical properties of wires occurs with decreasing wire diameter. The phenomena of ballistic transport of carriers, influence of the surface states on wire boundaries, orientation effects can be manifested even under the condition that diameter is found to be too large for the observation of the size quantization effect. All of these phenomena can significantly influence the charge transfer processes in nanowires [4].

InP system is of special interest for the investigation of nanowires due to low recombination rate of carriers on the surface states [5-7] and, thereby, has a considerable potential for the production of high-performance practical devices of optoelectronic direction.

The given work is devoted to the theoretical investigation of the band structure of deformed nanowires with different diameters. The results are important for the analysis of the charge transfer processes in photodetector devices based on InP nanowires and for the study of the radiative recombination in these materials.

2. CALCULATION TECHNIQUE

For the study of the features of the band structure of strained nanowires we have considered the model of deformed InP quantum wire in the form of a cylinder of length L and radius R (Fig. 1a). Based on the available experimental data [8], quantum wire is considered to be deformed (Fig. 1b). In the framework of the general approach to the calculation of deformations [9], we will choose distribution of components of the initial elastic displacements u_{i0} in the following form:

$$u_{x0} = u_0 \sin\left(\frac{\pi z}{L}\right),$$

$$u_{y0} = -\frac{2C_{12}}{C_{11}}, \quad (1)$$

$$u_{z0} = -\frac{2C_{13}}{C_{11}},$$

where C_{ij} are the tensor components of elastic constants; u_0 is the amplitude of the initial displacement.

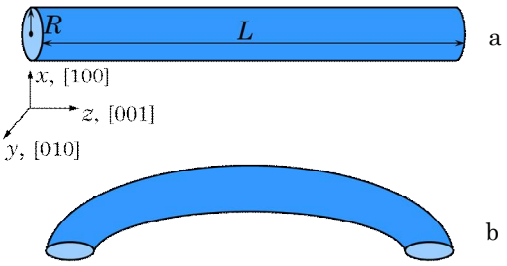

Fig. 1 – The studied InP quantum wire in the undeformed (a) and deformed (b) state

The appearance of deformations in quantum wires conditions the energy change of the conduction band bottom and valence band top by the values of δE_c and δE_v, respectively. In the approximation of deformation potential, shift of the energy band edges we will present as

$$\delta E_c = a_c \varepsilon_h + e\varphi, \quad (2)$$

$$\delta E_v = a_v \varepsilon_h - \frac{b_v}{2}\varepsilon_b + e\varphi, \quad (3)$$

where a_c, a_v, b_v are the deformation potential constants; φ is the piezoelectric potential; ε_h, ε_b are the hydrostatic and biaxial deformations which, in turn, are determined by the following correlations:

$$\varepsilon_h = \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z}, \quad (4)$$

$$\varepsilon_b = 2\frac{\partial u_z}{\partial z} - \frac{\partial u_x}{\partial x} - \frac{\partial u_y}{\partial y}. \quad (5)$$

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Distribution of the components of the elastic displacement vector u in the studied quantum wire was found by the solution of the system of equations of the theory of elasticity taking into account the piezoelectric properties of InP

$$\frac{\partial \sigma_{ij}}{\partial x_j} = 0, \quad \frac{\partial D_i}{\partial x_i} = 0\,, \tag{6}$$

where σ_{ij} is mechanical stress tensor; D_i is the electric flux which are connected with the deformation tensor and piezoelectric potential as follows

$$\begin{aligned} \sigma_{6\times1} &= C_{6\times6}\varepsilon_{6\times1} + e_{6\times3}\vec{\nabla}\varphi, \\ D_{6\times1} &= e_{3\times6}\varepsilon_{6\times1} - \nu_{3\times3}\vec{\nabla}\varphi. \end{aligned} \tag{7}$$

Here e and ν are the tensor components of piezoelectric and dielectric constants, respectively. Subscripts denote dimensions of the corresponding matrices.

System of equations (6)-(7) was solved numerically by the finite element method. Displacements u_i and piezoelectric potential φ obtained as a result of the solution were substituted into equations (4)-(5), and then changes of the energy bands (2)-(3) of InP quantum wire were calculated.

3. RESULTS AND DISCUSSION

In Fig. 2 we present the calculated changes of the energy band edges along the diameter of the strained InP wire for two end cross-sections of the quantum wire. As seen, deformation conditions the InP band gap change because of the shift of the conduction and valence band edges. Here, band gap in different sections of the nanowire can both increase (Fig. 2a) and decrease (Fig. 2b). We note that asymmetry of the band edge changes at $z = 0$ and $z = L$ is conditioned by nonsymmetrical behavior of the distribution of biaxial and hydrostatic deformations over cross-section along the Ox (Oy) axes.

Fig. 2 visually demonstrates that such deformation changes lead to the appearance of spatial local minima for free electrons in the conduction band and for holes in the valence band. In particular, a deep minimum in the conduction band inside the wire is found at $z = 0$ in the vicinity of $x = 33$ nm (Fig. 2a). Otherwise, at $z = L$ free electrons will be localized near the external edge of the wire (Fig. 2b).

The corresponding position changes of the conduction band bottom and valence band top along the axis of the quantum wire are illustrated in Fig.3. Again, minima for electrons and holes appear for real configuration of deformations inside the wire near its edges. Thus, a deep minimum for electrons appears near $z = 0$ and a local minimum on the other wire edge – at $z \approx$ 30-40 nm from the edge in depth. The last minimum is manifested for sufficiently small values of the wire diameter which are less than ≈ 10 nm in the considered case.

The presented data shows that spatially shifted local minima in the conduction and valence bands can appear in deformed wires. What is important is the fact that some of these minima are distant from the surfaces of the cylindrical wire (Fig. 2a and Fig. 3) with a usually substantial concentration of the charge carrier recombination centers. Blocking of the manifestation of these

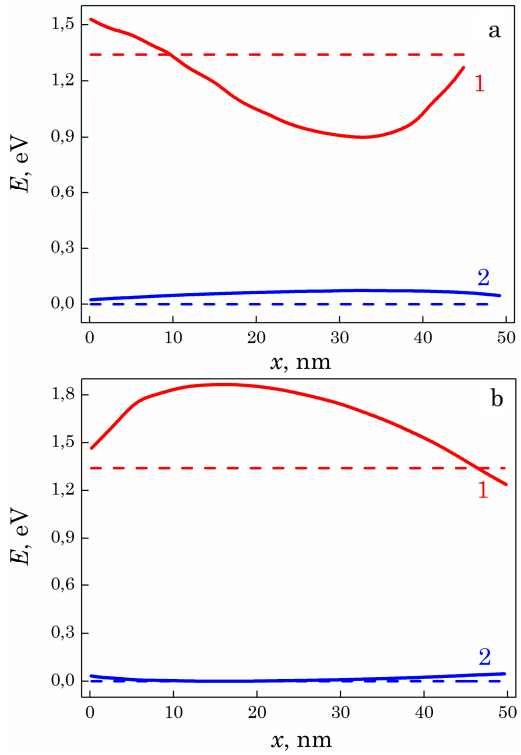

Fig. 2 – Deformation position changes of the conduction band bottom (1) and the valence band top (2) along the quantum wire diameter in different points: (a) – $z = 0$; (b) – $z = L$. Dashed lines denote the band edges in the undeformed wire. Wire radius is $R = 25$ nm, wire length is $L = 500$ nm

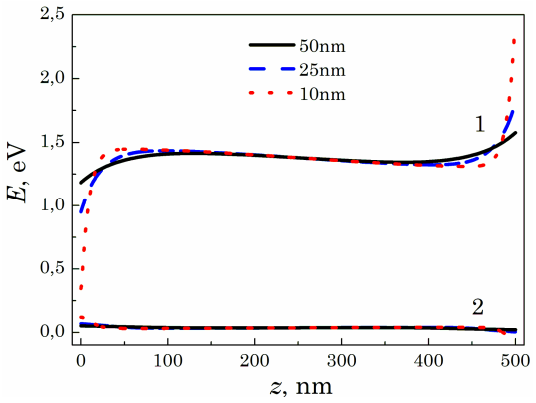

Fig. 3 – Deformation position changes of the conduction band bottom (1) and the valence band top (2) along the axis of the quantum wire of the length $L = 500$ nm for three values of the quantum wire radius (10, 25 and 50 nm)

centers with a significant enhancement of the charge carrier lifetime is mostly performed by functionalization of the wire surface, for example, by the coating with a polymer shell [10]. The given work proposes an alternative way, namely, partial blocking of the near-surface recombination by moving away of free carriers from the wire surfaces during its bending.

Thus, it is theoretically shown in the work that bending of quantum wires is able to create local minima in the conduction and the valence bands moved away from the surfaces of the cylindrical wire. This result gives new possibilities to control the lifetime of photoexcited charge carriers by keeping them in these minima and the photovoltage value in the solar cell conversion devices based on quantum wires.

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