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Elastic deformations distribution in laterally bent conical nanowires

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The elastic deformations in the conical nanowires are considered. An analytical expression was obtained for the distribution of elastic deformations along the length of the conical nanowire. It was found that at certain cone angles in nanowire there is an extended area of sufficiently high deformations comparable or even large than the deformation at the base of the nanowire. So, for example, when bending the conical (conical coefficient $a = -0.7$) nanowire with length $L = 1\,\mu$m and radius $R = 50$ nm by $\Delta z = 200$ nm, the maximum deformation values are $\varepsilon_{xx,\max} = 8\%$, while more than 95% of the nanowire is deformed by $> 3\%$.

Keywords: nanowires, elastic deformations, conical nanowires, Young's modulus.

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1. Introduction

In recent years, profound interest is attracted the study of the effect of mechanical deformations on the optical and transport properties of semiconductor nanostructures. When semiconductor nanowires (NW) are bent, significant elastic deformations (up to 11% [1]) can be observed in them, while the nanowires themselves do not break. This behavior under bendings differs significantly from the bendings of bulk materials, in which fracture occurs already at deformation $\sim 1\%$. The second important feature of thin nanowires is that the force required for their significant bending is quite small and can be only a few nanoNewtons. In the recent work [2] it was demonstrated that the bending of $In_xGa_{1-x}As$ ($x = 0.85$) nanowires by SPM-probe can lead to the increase in conductivity by several orders of magnitude. This offers opportunities for creating sensitive sensors and switches based on $In_xGa_{1-x}As$ nanowires. It should be noted that when cylindrical $In_xGa_{1-x}As$ nanowires are bent by an atomic force microscope probe, the region with increased conductivity [2] appears in the elastically deformable layer, which is due to the shift in position of the bottom of conduction band. In the case of bending cylindrical nanowires, the value of axial elastic deformations ε_{xx} is maximal at the base of the nanowire and linearly decreases $\varepsilon_{xx} \sim (1 - x)$ to zero at the point of application of the force ($x = 1$). Such decrease in deformations leads to the fact that at insufficiently high concentrations of indium in cylindrical $In_xGa_{1-x}As$ nanowires, conductivity switching may not occur. In this work, search for the optimal form to control the distribution of elastic strains in nanowires to increase the switchover performance of conductivity, was performed

2. Results

Fig. 1 shows the image of conical nanowires obtained using scanning electron microscopy (see Fig. 1, a), as well as the implementation scheme for lateral bends of nanowires by atomic force microscope probe (see Fig. 1, b). It should be noted that in a number of works [2–4] experiments were carried out on controlled lateral bending of cylindrical nanowires using the atomic force microscope probe. In this paper, within the Euler–Bernoulli theory of elasticity, we study the distribution of axial elastic strains along the length of bent conical nanowire.

It is worth making some remarks about the role of shear deformations in the analysis of nanowire bends. Indeed,

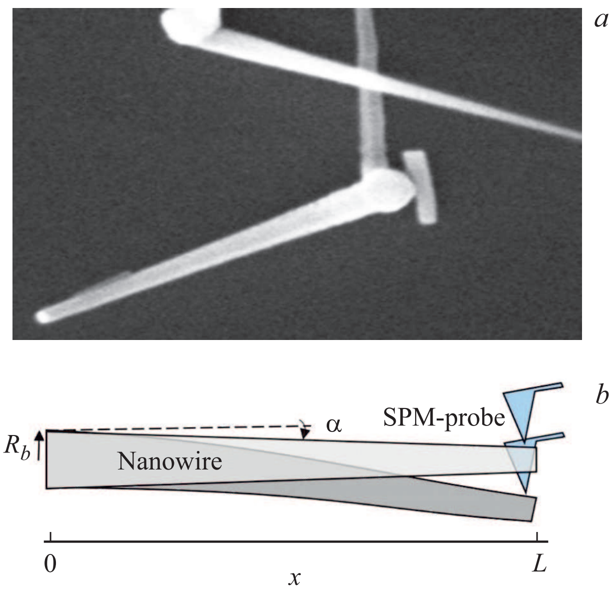

Figure 1. a — SEM image of conical nanowires with conicity coefficients $a = -0.8$ and $a = -0.5$; b — diagram of the bends of the conical nanowire.

in the general case, when beams are bent, both bending deformations and shear ones take place. To take into account shear deformations, it is necessary to move from the Euler–Bernoulli theory (which does not take into account shear deformations) to the equations of the Timoshenko theory. In Timoshenko's theory, the additional summand arises proportional to $\sim (E/G)\cdot(I/SL^2)$, where E is Young's modulus of the beam, G is beam shear modulus, I is second moment of beam section area, S is beam section area, L is beam length. In the case of long and thin nanowires, this summand turns out to be small, $\sim R^2/L^2$ (where R is the characteristic nanowire radius). Indeed, for most nanowires the ratio $R^2/L^2 < 1/100$, i.e. the correction summand associated with allowance for shear deformations turns out to be sufficiently small. This consideration determines the application of the Euler–Bernoulli model in this work.

The Euler-Bernoulli equation (1) together with the boundary conditions (2) makes it possible to determine the distribution $w(x)$ of bendings and axial deformations $\varepsilon_{xx}(x)$ along the length of a bent conical NW:

$$\frac{d^2}{dx^2}\left(EI(x)w''x\right) = 0, \tag{1}$$

$$w|_{x=0} = w'|_{x=0} = w''|_{x=L} = w'''|_{x=L} + \frac{F}{EI(L)} = 0. \tag{2}$$

Here E is Young's modulus of nanowire, $I(x)$ is moment of inertia of conical nanowire, L is length of nanowire. For conical NW with a conic angle α and base radius R_b, the following 2nd order differential equation can be obtained:

$$E\,\frac{\pi R_b^4}{4}\left(1+\frac{\alpha}{R_b}x\right)^4\frac{d^2w(x)}{dx^2} = F(L-x). \tag{3}$$

The values of axial deformations ε_{xx} inside the nanowire increase linearly from the axis to the edges. Near the axis, the deformation value ε_{xx} is equal to zero, and along the edges of the nanowire, the deformations have different signs (one side of the nanowire is compressed, while the other is stretched) and reach the maximum values $\varepsilon_{xx,\max}$:

$$\varepsilon_{xx,\max}(x) = \pm\frac{R(x)}{\rho(x)}. \tag{4}$$

Here $\rho(x)$ is the radius of curvature of the bent nanowire at the point x. Using formulas (3) and (4), as well as introducing the dimensionless coordinate $\xi = x/L$, the deformation at the base of the NW $\varepsilon_b = (F/E)(4/\pi R_b^3)L$ and the reduced conicity parameter $a = \alpha L/R_b$, we obtain the expression for $\varepsilon_{xx,\max}$

$$\varepsilon_{xx,\max}(\xi) = \varepsilon_b\,\frac{1-\xi}{(1+a\xi)^3}. \tag{5}$$

Fig. 2 shows the calculated profiles of normalized deformations $\varepsilon(\xi)/\varepsilon_b$ for conical nanowires with conicity coefficient $a = 0$ (solid curve), $a = -0.3$ (dashed curve), $a = -0.5$ (dashed curve), $a = -0.7$ (dot-and-dash curve). It can be

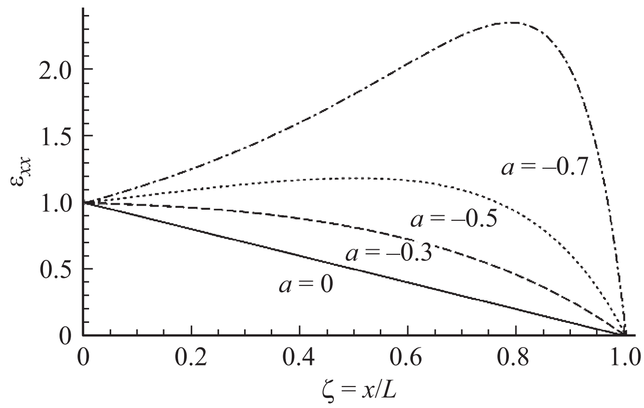

Figure 2. Normalized deformation profiles $\varepsilon(\xi)/\varepsilon_b$ for conical nanowires with conicity coefficients $a = 0$ (solid curve), $a = -0.3$ (dashed curve), $a = -0.5$ (dotted curve), $a = -0.7$ (dash-dotted curve).

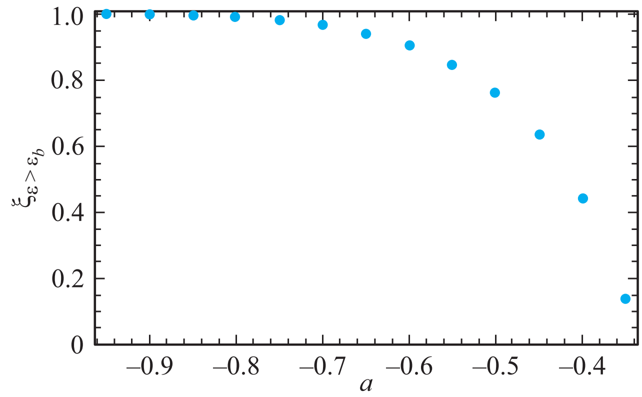

Figure 3. Dependence of the reduced length $\xi_{\varepsilon>\varepsilon b}$ of heavily deformed nanowire section on the conicity coefficient a.

seen that with a sufficiently strong conicity ($a < -0.3$), the extended region with deformations greater than ε_b appears in the NW. This situation is qualitatively different from the situation of cylindrical NW ($a = 0$) or „weakly conical“ NW ($a > -0.3$), when the greatest deformations and stresses occur only at the NW base. This property can improve the conductance switchover performance in devices based on conical NW [2]. Indeed, in the case of lateral bends of a conical InGaAs NW (with conicity coefficient of $a < -0.7$), the rather long conducting channel appears on the NW surface up to the contact region probe-NW.

Of particular interest is the question: which part of the nanowire is subject to deformations greater than the deformation at the base ($\varepsilon > \varepsilon_b$). A detailed view of the dependence of the size of the region of strong deformations on the conicity coefficient is shown in Fig. 3. The reduced length $\xi_{\varepsilon>\varepsilon_b}$ of strongly deformed section of the nanowire is plotted along the Y-axis. It can be seen that at low conicity coefficients ($-0.3 < a < 0$) there is no such region, at $a = -0.52$ the heavily deformed section occupies 80% of the nanowire, at $a = -0.6$ this section occupies 90%

of the nanowire, and at $a < -0.654$ this section already occupies more than 95% of the nanowire. Nanowires of this kind (with conicity coefficient of $a < -0.65$) can be promising structures for conductance switchover during lateral bending. So, for example, when bending the conical (conical coefficient $a = -0.7$) nanowire with length $L = 1\,\mu$m and radius $R = 50$ nm by $\Delta z = 200$ nm, the maximum deformation values are $\varepsilon_{xx,\max} = 8\%$, while more than 95% of the nanowire is deformed by $> 3\%$.

3. Conclusion

In this work, elastic deformations in conical nanowires are considered. The performed calculations show that the distribution of elastic deformations in conical nanowires differs significantly from the situation in cylindrical nanowires. Analytical expression is obtained for the distribution of elastic deformations along the length of conical nanowire It has been found that at certain conicity angles, the extended region of sufficiently high deformations arises in nanowires, comparable to or even greater than the deformation at the base. At sufficiently high conicity angles, the region of high deformations covers almost the entire length of the nanowire, which makes it possible to more performantly switch the conductivity in such nanowires. So, for example, when bending the conical (conical coefficient $a = -0.7$) nanowire with length $L = 1\,\mu$m and radius $R = 50$ nm by $\Delta z = 200$ nm, the maximum deformation values are $\varepsilon_{xx,\max} = 8\%$, while more than 95% of the nanowire is deformed by $> 3\%$.

Conflict of interest

The authors declare that they have no conflict of interest.

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