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# Study of elastic deformations in tapered nanowires

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**Abstract**. In this work, the calculation of the values of elastic deformations and stresses arising in tapered nanowires is carried out. It was found that in tapered nanowires the magnitude of deformations changes from the base of the nanowire to its tip not linearly (as would be the case in cylindrical nanowires), but in a more complex manner. The ranges of conicity angles at which an extended region of increased stresses can appear in tapered nanowires have been determined.

## 1. Introduction

In recent years, the study of the impact of mechanical deformations on the optical and transport properties of semiconductor nanowires (NW) has been of great interest. Bending nanowires can lead to significant elastic deformations (up to 11% [1]), which significantly distinguishes this situation from that in bulk materials. The second important feature of thin nanowires is that the force required to bend them could be as small as only a few nanonewtons. In recent work [2], it was demonstrated that the $In_xGa_{1-x}As$ (x=0.85) nanowires bending by an SPM-probe can lead to several orders of magnitude increase in conductivity of thin NWs. This opens up the possibility of creating sensitive switches and sensors based on $In_xGa_{1-x}As$ nanowires.

It should be noted that, when cylindrical nanowires are bent by an SPM probe, an elastically deformable layer with increased conductivity (which is due to a shift in the position of the conduction band bottom [2]) appears on the surface. In this case, the value of axial elastic deformations $\varepsilon_{xx}$ is maximum at the base of the nanowire and linearly decreases $\varepsilon_{xx}$~(L-x) down to zero at the point of application of the force (x=L). This decrease in deformations leads to the fact that, at insufficiently high indium concentrations in $In_xGa_{1-x}As$ nanowires, conductivity switching may not occur. In this work, the search for the optimal shape for controlling the distribution of elastic deformations in the nanowire and increasing the efficiency of switching conductivity in nanowires is carried out.

In this work, we will consider tapered nanowires. It will be shown below that in such nanowires it is possible to create extended regions with sufficiently large axial deformations $\varepsilon_{xx}$ due to relatively small bends. It should be noted that tapered shaped nanowires are quite often obtained during growth by the vapour-liquid-solid mechanism [3], that is, the situation under consideration is not exotic one.

## 2. Results and discussion

Figure 1 shows a typical SEM image of conical nanowires (see Figure 1b) and a scheme of nanowire bending (see Figure 1a). It should be noted that experiments with controlled bending of nanowires with an SPM probe were carried out in the works [2,3,4]. In this work, we will investigate the distribution of axial elastic deformations along the length of a bent tapered nanowire in the framework of the elasticity theory.

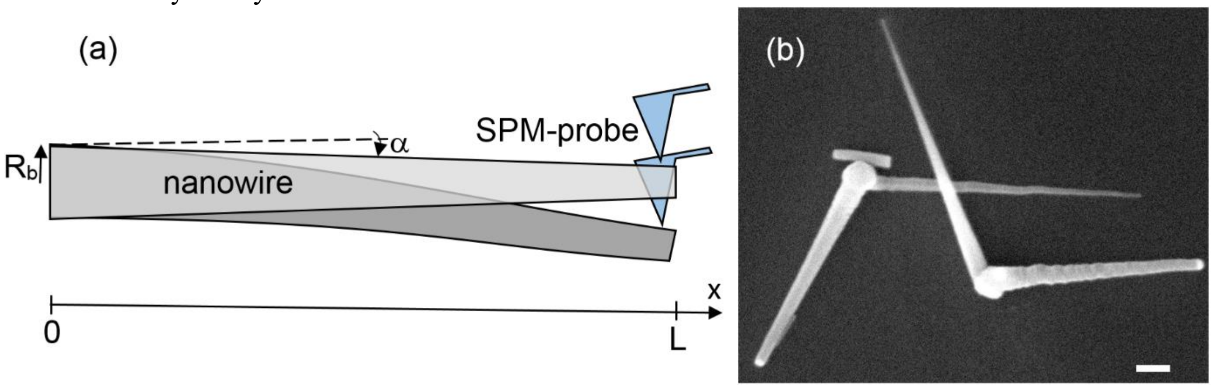


**Figure 1.** (a) – Scheme of tapered nanowire bending; (b) – Scanning electron microscopy image of tapered nanowires with conicity coefficient ranging from -0.9 to -0.5.

The Euler-Bernoulli equation (1) together with the boundary conditions (1a-1d) makes it possible to determine the distribution w(x) of bends and axial deformations $\varepsilon_{xx}(x)$ along the length of the conical nanowire.

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

$$w\Big|_{x=0} = 0 \tag{1a}$$

$$\frac{dw}{dx}\Big|_{x=0} = 0 \tag{1b}$$

$$\frac{d^2w}{dx^2}\Big|_{x=L} = 0 \tag{1c}$$

$$\frac{d^3w}{dx^3}\Big|_{x=L} = \frac{-F}{EI(L)} \tag{1d}$$

Where E is the nanowire Young's modulus, I(x) is the second area moment of inertia of the tapered nanowire, L is the length of NW. Using (1.c) and (1.d) boundary conditions one can obtain the following second order differential equation:

$$EI(x)\frac{d^2w(x)}{dx^2} = F(L-x) \tag{2}$$

For the tapered NW with the cone angle tangent α and base radius $R_b$ the I(x) is given by the following relation:

$$I(x) = \frac{\pi R_b{}^4}{4}(1+\frac{\alpha}{R_b}x)^4 \tag{3}$$

The values of axial deformations $\varepsilon_{xx}$ inside the nanowire are linearly distributed from the center to the edges. Near the center of nanowire the deformation $\varepsilon_{xx}$ value is zero, and at the nanowire edges the deformations have different signs (one side of the nanowire is compressed while the opposite side is stretched) and reach maximum values $\varepsilon_{xx,max}$:

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

Here ρ(x) is the radius of curvature of the bent nanowire at the point x. In what follows, we will be interested only in the absolute value of the maximum value of axial deformations $\varepsilon(x)=|\varepsilon_{xx,max}(x)|$ at the edge of the nanowire. Using formulas (2) and (3), as well as an approximate expression for the radius of curvature of the nanowire $\rho(x) = d^2w(x)/dx^2$, we obtain the expression for ε(x):

$$\varepsilon(x) = \frac{F}{E}\frac{4}{\pi R_b{}^3}\frac{L-x}{(1+\alpha x/R_b)^3} \tag{5}$$

Expression (5) can be simplified by introducing the dimensionless coordinate ξ=x/L, deformation at the base of the nanowire $\varepsilon_b=(F/E)(4/\pi R_b^3)L$, and the reduced conicity parameter $a=\alpha L/R_b$:

$$\varepsilon(\xi) = \varepsilon_b \frac{1-\xi}{(1+a\xi)^3} \tag{6}$$

Figure 2 shows the calculated profiles of the values of normalized deformations $\varepsilon(\xi)/\varepsilon_b$ for tapered nanowires with a conicity coefficient a=0 (black curve), a=-0.3 (red curve), a=-0.5 (blue curve), a=-0.7 (green curve). It can be seen that, at a sufficiently strong conicity (a<-0.3), an extended region with deformations greater than $\varepsilon_b$ appears in the nanowire. This situation is qualitatively different from the situation of a cylindrical nanowire (a=0) or a “weakly conical” nanowire with -0.3<a<0, when the greatest deformations and stresses arise only at the base of the nanowire. This property can improve the efficiency of conductivity switches based on tapered nanowires [2]. Indeed, in the case of lateral bends of a tapered InGaAs nanowire (with a <-0.7), a sufficiently long conducting channel will appear on the nanowire surface up to the probe-nanowire contact region. It should be noted that nanowires with such a conicity are quite common. For example, the values of the conicity parameter “a” for the nanowires shown in Figure 1b range from -0.9 to -0.5 (i.e., the radius of the nanowires from the base to the tip changes by 50-90%). Thus, the bends of such tapered nanowires should lead to the appearance of extended strongly deformed region, which will make it possible to effectively switch the conductivity in such nanowires.

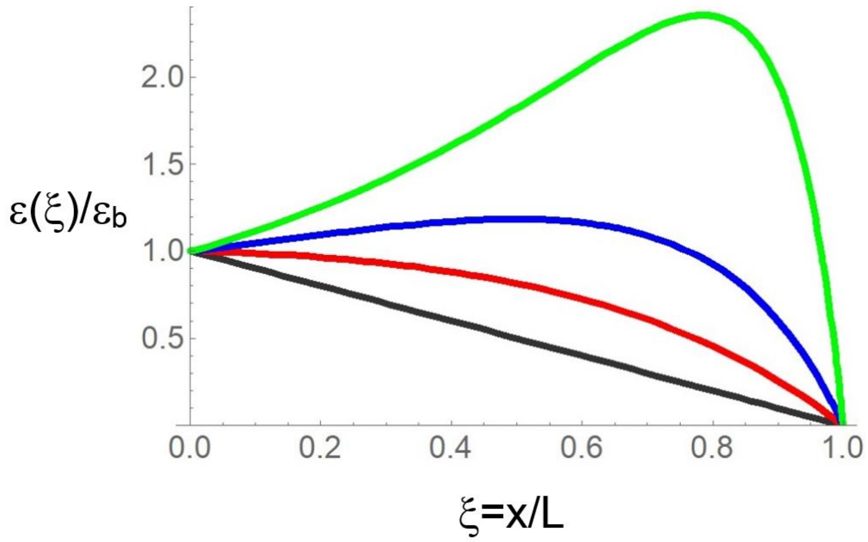


**Figure 2.** Normalized deformation $\varepsilon(\xi)/\varepsilon_b$ profiles for tapered nanowires with a conicity coefficients a=0 (black curve), a=-0.3 (red curve), a=-0.5 (blue curve), a=-0.7 (green curve).

It is also worth noting that in tapered nanowires with a sufficiently strong conicity (a<-0.5), at a certain distance from the base, a region appears in which elastic strains and stresses are multiples of the strains and stresses at the base of the nanowire (see the green curve in Figure 2). The presence of such strongly deformed regions may be of interest when studying the dependence of the optical properties of materials on the values of elastic stresses. When the tapered nanowires are deformed with an SPM probe, it is possible to study the Raman spectra and shifts of photoluminescence lines. An analysis of the Raman spectra makes it possible to refine the values of elastic stresses in bent nanowires. The shift of the lines in the photoluminescence spectra makes it possible to determine the magnitude of the shifts of the edges of the conduction and valence bands upon deformation. That is, working with tapered nanowires provides a unique opportunity to achieve high values of elastic deformations and stresses at sufficiently small deformations. The authors plan in the future to carry out such optical experiments on nanowires with a strong conicity.

## 3. Conclusion

The calculations performed in this work show that the distribution of elastic deformations in tapered nanowires is significantly different from the situation in cylindrical nanowires. An analytical expression is obtained for the distribution of elastic strains along the length of a tapered nanowire. It was found that at certain angles of conicity in nanowires, an extended region of sufficiently high deformations, comparable or even greater than the deformation at the base of the nanowire, can arise. At sufficiently high conicity angles, the region of high deformations covers almost the entire length of the nanowire, which makes it possible to more efficiently switch the conductivity in such nanowires.

## References

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