Two-dimension curvature of a wire: A simple model using shear modulus concept

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Abstract

In this work simple model based on definition of shear modulus to produce bending of wire is proposed. Several results are discussed only for constant shear modulus and diameter, but the model can be extened to non-constant shear modulus and diameter. For arbitrary parameters the model can show bending of wire which depends on shear modulus, wire mass, initial angle, and number of segments. Unfortunatey, it does not give fully agreement for nanowire system, which produces higher value than expected.

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1 Introduction

It is interesting to calculate how the curvature of a wire with not constant elastic modulus due to influence of gravitation, where the formulation for bending sparklers has been proposed previously (Abdullah et al., 2014). In general a wire has constant shear modulus even when the diameter is not constant. In nanoscale system it is very different as observed in ZnO nanowires. Tangential shear modulus observed using contact resonance atomic force microscopy shows a pronounced increase when diameter of [0001] ZnO nanowire is reduced below 80 nm (Stan et al., 2007). ZnO nanowires 60-30 nm diameter and a typical length of 2 μm gives Young's modulus within 30% of that of bulk as manipulated with an atomic force microscopy tip mounted on a nanomanipulator inside a scanning electron microscope (Hoffmann et al., 2007). Young's modulus of [0001] oriented ZnO nanowires with diameters 17-550 nm increases dramatically for diameter smaller than about 120 nm with decreasing diameters and significanly higher than the larger ones whose modulus tends to that of bulk ZnO (Chen et al. 2006). The [0001] ZnO has maximum Young's modulus ~ 249 GPa for d = 40 nm for range 40-110 nm, but not observed for range 200-400 nm, where has only an average constant of value ~ 147.3 GPa, close to the modulus value of bulk ZnO. It also observed that thick ZnO nanowires (d > 200 nm) were brittle, while the thin nanowires (d < 110 nm) were highly flexible (Asthana et al., 2011).

2 Theory

A solid with length *L* and cross section area *A* can be deformed by force *F* applied parallel to the area A as shown in Figure 1.

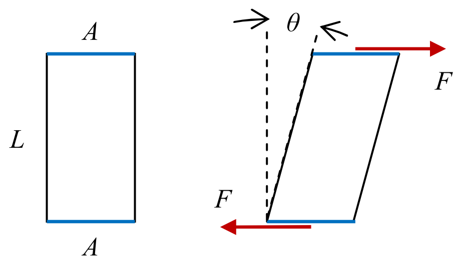

Figure 1. Force *F* parallel to area *A* gives deformation of angle *θ* to length *L*.

Shear modulus *G* is defined as

$$G = \frac{F / A}{\theta}, \tag{1}$$

where

$$\frac{\Delta x}{L} = \tan\theta \approx \sin\theta \approx \theta \tag{2}$$

for small angle. A wire can be constructed from several segments with length ΔL and a segment i will have angle difference $\Delta\theta_i$ from preceding segment i–1.

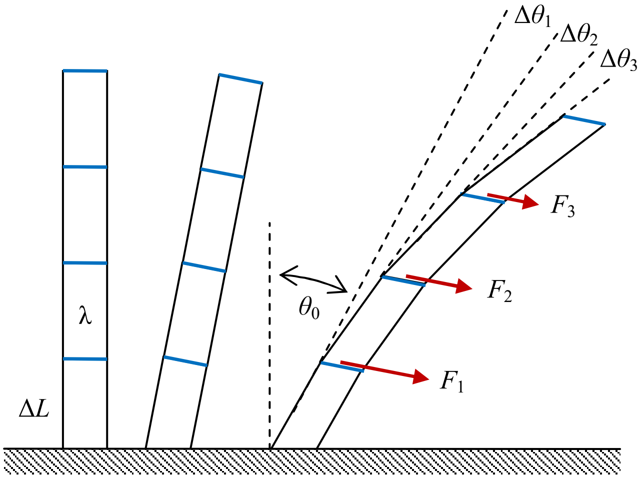

Figure 2. Wire with θ_0 = 0 (left), wire with very high value of G (center), and wire with certain curvature (right).

Suppose that a wire with mass M and length L will have mass density ρ

$$\rho = \frac{dm}{dV}, \tag{3}$$

where l is coordinate along wire length. Mass M will be obtained from

$$M = \int dm = \int_0^L \rho \, dA \, dl, \tag{4}$$

with

$$dA = 2\pi r dr, \tag{5}$$

where $r = r(l)$. At position l lower segment will have force F in a form of

$$F = g\sin\theta \int_l^L 2\pi\rho\, r dr\, dl = \pi\rho g \sin\theta \int_l^L r^2 \, dl. \tag{6}$$

Using Equation (1) it can be obtained that

$$\Delta\theta = \frac{\rho g \sin\theta}{r^2 G} \int_l^L r^2 dl, \tag{7}$$

where $\theta = \theta(l)$ and $A = A(l)$. Equation (6) can be written in following form

$$\theta(l+\Delta l) = \theta(l) + \rho g \frac{\sin\theta(l)}{G(l) r^2(l)} \int_l^L r^2(l) dl, \tag{8}$$

which depends on $\theta(0)$. Case for $\theta(0) = 0$ is given in Figure 2 (left). The wire will have trajectory

$$x(l+\Delta l) = x(l) + \Delta L \sin\theta(l) \tag{9}$$

$$y(l+\Delta l) = y(l) + \Delta L \cos\theta(l), \tag{10}$$

where $x(0) = x_0$ and $y(0) = y_0$ is the origin. Step along the length Δl depends on number of segments N through

$$\Delta l = \frac{L}{N}, \tag{11}$$

which should be carefully chosen that is not so many but already change the curvature when the value is increased. Error can defined as

$$\varepsilon_N = \sum_{\substack{i=0,\\ j=2i}}^{N} \left[x(l_i) - x(l_j)\right]^2 + \left[y(l_i) - y(l_j)\right]^2 \tag{12}$$

with

$$l_i = i\Delta l_i, \quad i = 0,..,N, \quad \Delta l_i = \frac{L}{N}, \tag{13.a}$$

$$l_j = j\Delta l_j, \quad j = 0,..,2,N \quad \Delta l_j = \frac{L}{2N}. \tag{13.b}$$

Every position of segment $[x(l_i), y(l_i)]$ with number of segments N is compared to every position of segment $[x(l_j), y(l_j)]$ with number of segments $2N$ at the same position. Or the simpler expression could be

$$\varepsilon_N = \sum_{\substack{i=0,\\ j=2i}}^{N} \left[\theta(l_i) - \theta(l_j)\right]^2 . \tag{14}$$

Minimum value of ε_N can be found if

$$\frac{\partial \varepsilon_N}{\partial N} = 0 \tag{15}$$

can be formulated and calculated. A parameter known as tortuosity T is defined as follow

$$T = \frac{1}{L}\sqrt{(x_N - x_0)^2 + (y_N - y_0)^2} \tag{16}$$

in this case.

Table 1. Calculation parameters.

Parameter	Unit	Value	References
ρ	g/cm^3	5.606	Zhu *et al.* (2009)
D	nm	40–400	Asthana *et al.* (2011)
	μm	200–300	Kim *et al.* (2014)
G	GPa	147.3–249*	Asthana *et al.* (2011)
	GPa	67.5–79.4	Kim *et al.* (2014)
L	μm	2–6	Xu *et al.* (2008)
	μm	1.8	Kim *et al.* (2014)
g	m/s^2	9.78	Fukuda *et al.* (2004)

*In reverse trend with D

Comparing maximum length and minimum diameter from Table 1 value of 50 is obtained, which can be considered as ratio of L/D.

3 Results and discussion

3.1 Arbitrary parameters

In order to see how how parameters influence bending of the wire, following values are used $\theta_0 = 10°$, $L = 1$ m, $M = 2$–22 g, $D = 2$ mm, $G = 2.5\times10^4$–10^5 N/m^2, $N = 5$–80. Figure 3 shows that higher value of N gives more curved wire.

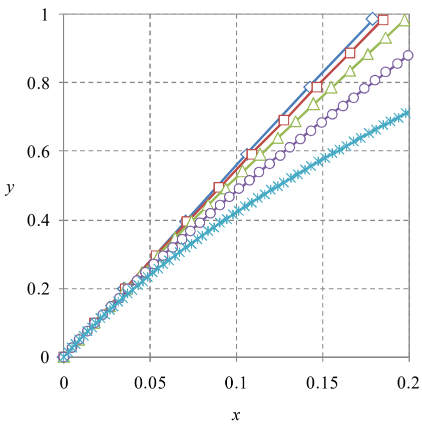

Figure 3. Curvature of wire with $\theta_0 = 10°$, $L = 1$ m, $M = 10$ g, $D = 2$ mm, $G = 10^5$ N/m^2 for several values of N: 5 (◊), 10 (□), 20 (△), 40 (○), and 80 (×).

This is different than influence of G, where higher value of G gives more stright curvature thatn the lower ones as shown in Figure 4 and there is also a certain value of G which gives minimum value of tortuosity T.

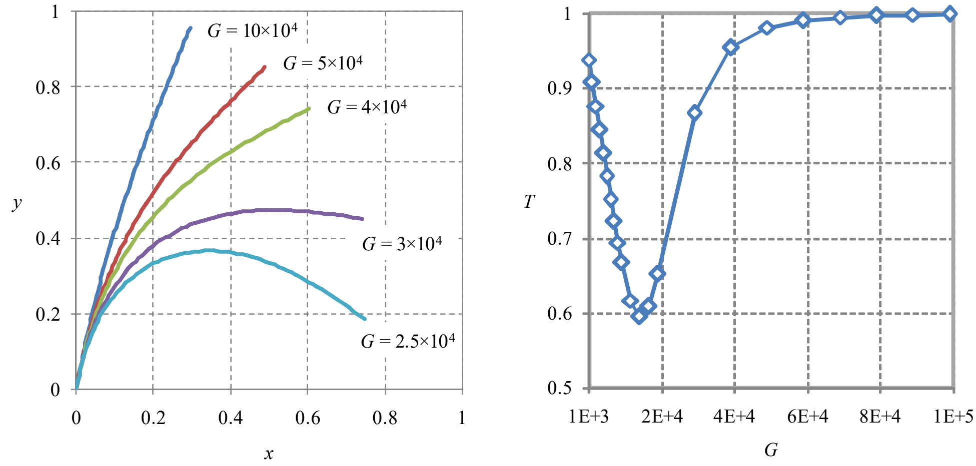

Figure 4. Curvature of wire with θ_0 = 10°, L = 1 m, M = 10 g, D = 2 mm, N = 80 for several values of G (left) and its tortuosity T as function of G in N/m^2 (right).

As shear modulus G getting smaller turtuosity will reduce to until a minimum value and it begins to increase again. For given parameters minimum tortuosity Tmin is obtained at G about 1.5×10^4 N/m^2.

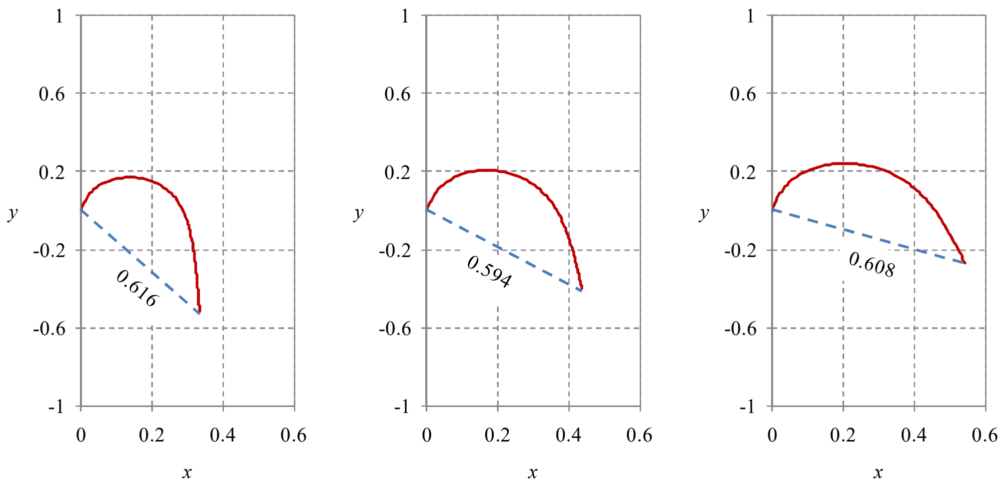

Figure 5. Curvature of wire with θ_0 = 10°, L = 1 m, M = 10 g, D = 2 mm, N = 80 for several values of G: 1.25×10^4 (left), 1.5×10^4 (center), 1.75×10^4 (right), where minimum tortuosity T_{min} is given by $G \approx 1.5\times10^4$ N/m^2.

Wire with heavier mass M tends to bend more compared to the lighter one as seen in Figure 6.

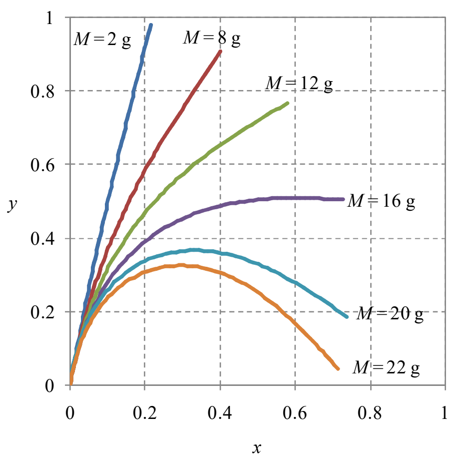

Figure 6. Curvature of wire with θ_0 = 10°, L = 1 m, G = 5×10^4 N/m^2, D = 2 mm, N = 80 for several values of M.

3.2 Nanowire parameters

In this part parameters in the ranges from Table 1 are used. As sample two nanowires from SEM images (Liu *et al*., 2008) is roughly digitized and assumed linear as shown in Figure 7. There are also other nanowire size given in Figures 8 and 9, as reported by Kim *et al*. (2014) and Xu *et al*. (2008), respectively.

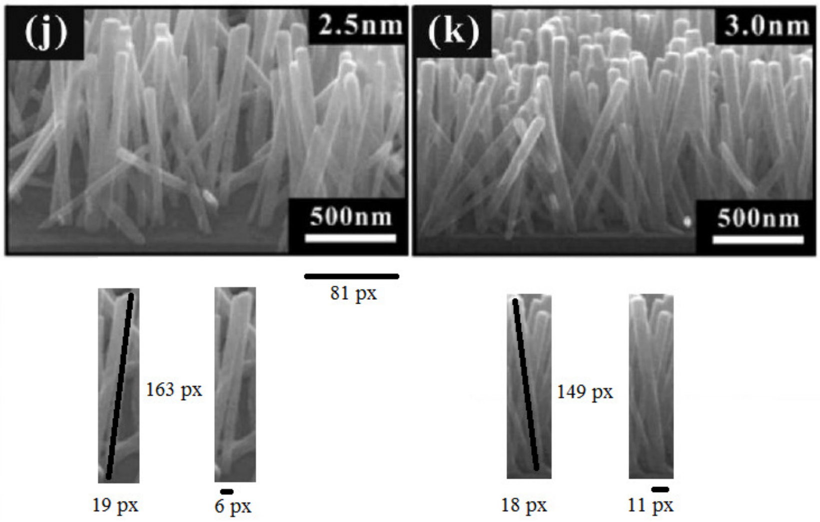

Figure 7. Rough digitation of nanowire from SEM images with different seed layer thickness (Liu *et al.*, 2008).

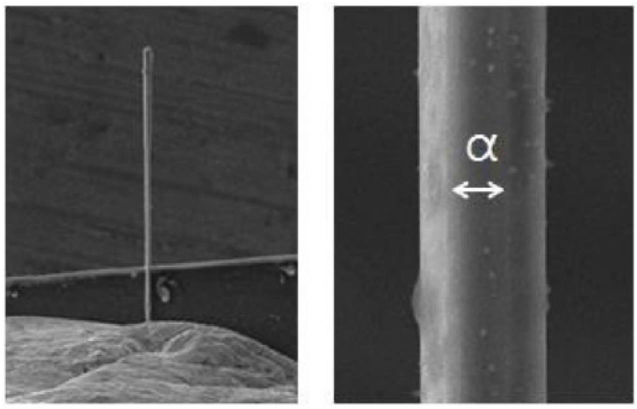

Figure 8. SEM images of single nanowire with length L = 84.5 μm and side width of the hexagonal structure α = 980 nm or D is about 1.8 μm (Kim *et al*., 2014), where $\Delta x \approx 1$ px and $\Delta y \approx 218$ px.

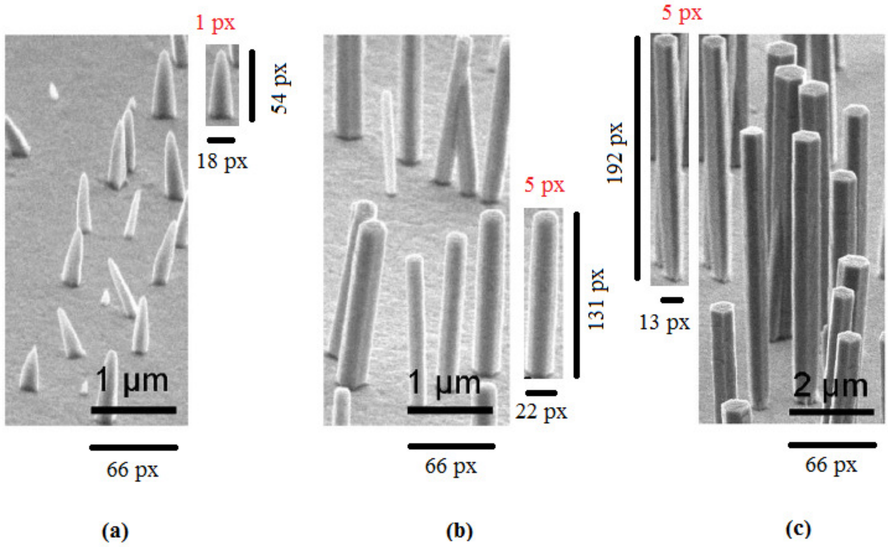

Figure 9. Growing of nanowire as observed using SEM at time t: (a) 0.5 h, (b) 6, and (c) 48 h, where growth domination is altered from lateral (t < 0.5 h), axial (0.5 h < t < 6 h), and both (6 h < t < 48 h), as reported (Xu *et al*., 2008).

Based on Figures 7-9 following parameters are using in calculations, which is assumed that all the wires are still straight ($\theta_N \approx \theta_0$) due to difficulties in digitizing the available SEM images. Condition of $\theta_N \approx \theta_0$ can be considered related to D / L.

Table 2. Nanowire parameters.

Figure	Reference	L (nm)	D (nm)	θ_0 (rad)	E (GPa)	D / L
7	Liu *et al.*, (2008)	1013	37	0.116	-	0.037
		926	67.9	0.121	-	0.073
8	Kim *et al.*, (2014)	84500	1800	0.005	67.5–79.4	0.021
9	Xu *et al.*, (2008)	818	272	0.019	-	0.333
		1986	333	0.038	-	0.168
		5820	394	0.026	-	0.068

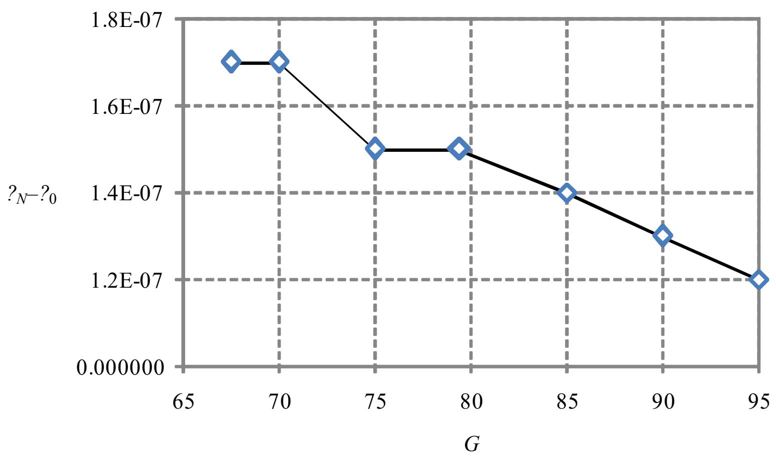

Figure 10. Difference between final and initial angle θ_N–θ_0 as function of shear modulus G.

By choosing $N = 10^6$ results in Figure 10 can be obtained, these differences are already quite small compare to value of initial angle θ_0. Using the relation

$$E = 2G(1+\nu), \tag{17}$$

And set Poisson ratio $\nu = 0$ it can be obtained results in Table 4.

Table 3. Young's modulus from calculated shear modulus.

Figure	Reference	E_{exp} (GPa)	E_{cal} (GPa)
7	Liu *et al.*, (2008)	-	> 17
		-	> 12
8	Kim *et al.*, (2014)	67.5–79.4	> 190
9	Xu *et al.*, (2008)	-	> 11
		-	> 26
		-	> 74

Table 3 shows that G can only be predicted for the minimum value, since value greater than the computed ones will give the same straight nanowire.

A nanowire with radius R_{NW}, shell thickness t, and core radius $R_c \equiv R_{NW} - t$, can have realistic Young's modulus E_{NW} (Stan et al., 2007)

$$\frac{R_{NW}}{E_{NW}} = \frac{t}{E_s} + \frac{R_c}{E_c} \tag{18}$$

from the analysis of strain under uniform radial stress condition, where E_c and E_s are Young's modulus of core and shell, respectively.

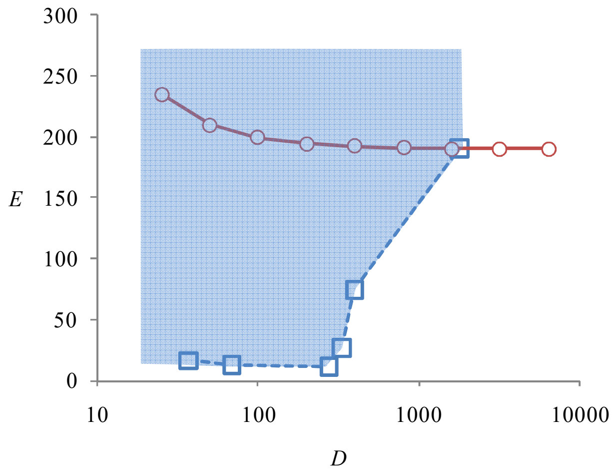

Figure 11. Young's modulus E (in GPa) as function of nanowire diameter D (in nm): calculation data (□) and from Equation (18) with E_s = 250 GPa, E_c = 190 GPa, and t = 10 nm (○), where blue-shaded area has lower boundary of calculation data.

Results of Young's modulus from Table 3 are only the minimum values, which means that they give only lower bound of E. Because of that, they can be superimposed with values obtained from Equation (18) as shown in Figure 11. Weakly since the model does not take into account hollow space in the nanowire, it can be said that calculation results in Table 1 are right since they are all lower than values from Equation (18) if values of E_s = 250 GPa, E_c = 190 GPa, and t = 10 nm are used.

3.3. Future plan

It is interesting to advance the proposed mode with hollow structure for a hollow wire with outter diameter D_o and inner diameter D_i (or shell thickness $2t \equiv D_o - D_i$), so that the results can be compared to Equation (18).

Conclusion

A simple model of wire bending derived from definition of shear modulus has been presented and can be used for arbitrary parameters but not so successful for the size of nanowire, since it predicts too higher value than measured in experiments, but could be rather good if the nanowire is not solid but a hollow one.

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