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Elasticity of DNA nanowires

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ABSTRACT

In this paper, we bring forth the Young modulus of DNA nanowire (NWs) as a function of diameter considering both equilibrium strain and surface stress effects. A good trend between the present calculated and the available theoretical size-dependent Young modulus of different NWs is found, which supports the DNA NWs mechanical strength. We have extended our view to predict the behavior of the DNA NWs and see their resemblance to the behavior of either metallic or semiconducting nature of NWs. We have also demonstrated the variation in Young modulus of the DNA NWs with the variation of relaxed material property of DNA NWs. This study extrapolates key factors in modeling DNA NWs for the electronic device applications.

1. Introduction

Deoxyribonucleic acid (DNA), well known for duplication and storage of genetic information in biology, has also recently been shown to be highly useful as an engineering material [1]. DNA being chemically robust and with exceptional length control is an effective template for formation of nanowires. Because of the highly specific nature offered by biomolecules such as DNA and RNA (ribonucleic acid) the nanostructures can be assembled into functional devices via bio-recognition-directed assembly method. The interaction between complementary DNA and reversible, enabling highly controlled assembly of nanostructures, makes DNA an important contestant for producing nanowires.

The intensive interest in DNA NWs exists because they exhibit the torsional and bending stiffness, differing them from simpler NWs [1]. Due to this, exclusive physical properties are observed which are better than in their complementary bulk counterparts. Several previous studies dealing with the elastic properties of NWs exist [2,3], but still an additional effort is required in order to systematically describe the dependence of the Young modulus on NW parameters [4].

A great influence on the overall mechanical properties of the NWs, believed to be determined by the contribution of both bulk elastic modulus and surface elastic modulus, is seen due to the diameter of these nanomaterials [5,6]. Maybe as a result of the differing diameters, the surface bonding [7] and observed nonlinear bulk phenomena [8], the relative increase or decrease in the elastic properties of these nanomaterials is seen. Since these DNA NWs have the diameters of the same order of magnitude as diameters of semiconductor nanocrystals or quantum dots, an analogy can be set for the elastic vibrations of the DNA NWs with those of the spherical quantum dots.

Typical DNA NWs are miniscule pockets of proteins and well known as a genetic material. Therefore, it is now interesting and important from both fundamental and application point of view to explore and study the Young modulus of the nanomaterials regarding their surface and bulk materials properties. In the present work, we focus on the mechanical properties of the DNA NWs, like Young modulus, along with relaxed/unrelaxed metal and semiconductor NWs. Further, we gain insight into the similarities of different properties of DNA NWs, which enables us to predict the nature and the application of DNA NWs. Thus, the applications of NWs in various fields of nanoscience can be increased as nanowires can be synthesized by keeping in mind the required properties and the effects of diameter on their properties.

2. Methodology

The total energy the nanowire can be expressed as a sum of the energy contributed from bulk and surface materials [3],

$$U = \frac{\pi (D-2t)^2}{4} L\Omega(\varepsilon) + \pi D L \gamma(\varepsilon), \tag{1}$$

where $\Omega(\varepsilon)$ is the bulk energy density in the nanowire core, $\gamma(\varepsilon)$ is the surface energy of the nanowire surface, D is the diameter of the nanowire, L is the length of the nanowire and t is the thickness of the nanowire.

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Table 1
Physical parameters used in this work (here a = relaxed and b = unrelaxed surfaces).

System	Young modulus E (GPa)	Poisson's ratio (ν)	Surface stress in J/m^2
Ag	79^a	0.37^a	0.27^a
	79^b	0.37^b	-0.773^b
Au	80^a	0.42^a	2.4^a
	80^b	0.42^b	-0.901^b
TiO_2	151^a	0.27^a	-1.2^a
	151^b	0.27^b	0.9^b
Si	130^a	0.29^a	-0.5^a
	130^b	0.29^b	1.38^b
DNA	0.3^a	0.5^a	-0.6^a

[a] Refs. [1,3,5,13].
[b] Refs. [3,5,9,13].

Let the nanowire be deformed by a strain δ from its equilibrium state due to some load (where ϵ^* is the equilibrium strain). Then, $\delta = \epsilon/(1+\epsilon^*)$ (here ϵ is the strain in accordance to the equilibrium crystal lattice). Hence, Young modulus contributed from the nanowire's core should be

$$\epsilon^* = \frac{E_s}{\frac{(D-2t)^2(E_s+E_b)}{4D}} \tag{2}$$

Here, E_s is the surface elastic modulus whereas E_b is the bulk elastic modulus. We know that surface stress ($g = \gamma + \mathrm{d}\gamma/\mathrm{d}\varepsilon$) is the reversible work per unit area required to elastically stretch a surface [9]. Total surface area of the nanowire changes by $\pi D(1-\nu)\Delta L$ (ν is Poisson's ratio) when a circular nanowire is subjected to a deformation [3]. This results with energy change that is associated with the surface deformation of the nanowire, given by $\Delta U_s = \pi D(1-\nu)g\Delta L$. It is also observed that the change in nanowire length (ΔL) is proportional to the square of the deflection under clamped-end three-point bending which is most often used to measure Young modulus of NWs [10–12]. Hence, the surface stress can be given by

$$g = \frac{5}{8}\frac{E_s}{(1-\nu)}\frac{D^3}{L^2} \tag{3}$$

We know that the Young modulus of the nanowire in terms of surface stress and diameter, as a sum of core and surface Young modulus from the above equations, is given as

$$E_{\text{nanowire}} = \left(1+\epsilon^*\right)^2 E_b + \frac{8}{5}g(1-\nu)\frac{L^2}{D^3} \tag{4}$$

As the diameter of NWs increases, the equilibrium strain approaches zero according to Eq. (3). Therefore, when D reaches the limit of bulk materials E_{nanowire} would be equal to the bulk modulus (E_b). Consequently, it is the elastic modulus of infinitely large extended surface, and ϵ^* is the strain at which the surface energy reaches its minimum.

3. Results and discussion

Our results are based on the behavior of the Young modulus of DNA NWs. We will discuss the behavior of DNA nanowires with decreasing diameters and their resemblance with either metallic or semiconducting behavior of the NWs. In our study length of the nanowire is assumed to be 1000 nm, the typical length when the nanowire is suspended using three point's clamped bending condition [3,4].

3.1. Metallic and semiconductor nanowires

In order to understand the behavior of the DNA NWs, we have theoretically estimated the behavior of metallic and semiconductor NWs under both relaxed and unrelaxed conditions. Figs. 1 and 2 show the comparison of Young moduli in metallic (Ag and Au) and semiconductor (TiO_2 and Si) nanowires in fully relaxed and unrelaxed conditions, respectively. Calculated physical parameters are presented in Table 1. From our calculations on relaxed NWs (Fig. 1) it can be seen that there is an increase in the Young modulus for metallic NWs and a decrease in the Young modulus of semiconductor NWs with decreasing diameter. This effect of increase or decrease in Young modulus is primarily due to the surface stress (Eqs. (3) and (4)). Surface stress is positive for relaxed metallic NWs [3], while, on the other hand, it is negative for relaxed semiconductor NWs [14]. For the unrelaxed conditions the behavior shown by both types of specimens is reversed as shown in Fig. 2. As the surface stress is negative for unrelaxed metallic NWs and positive for unrelaxed semiconductor NWs, metallic NWs show a significant decrease, while semiconductor NWs show an increase in the Young modulus with decreasing diameters.

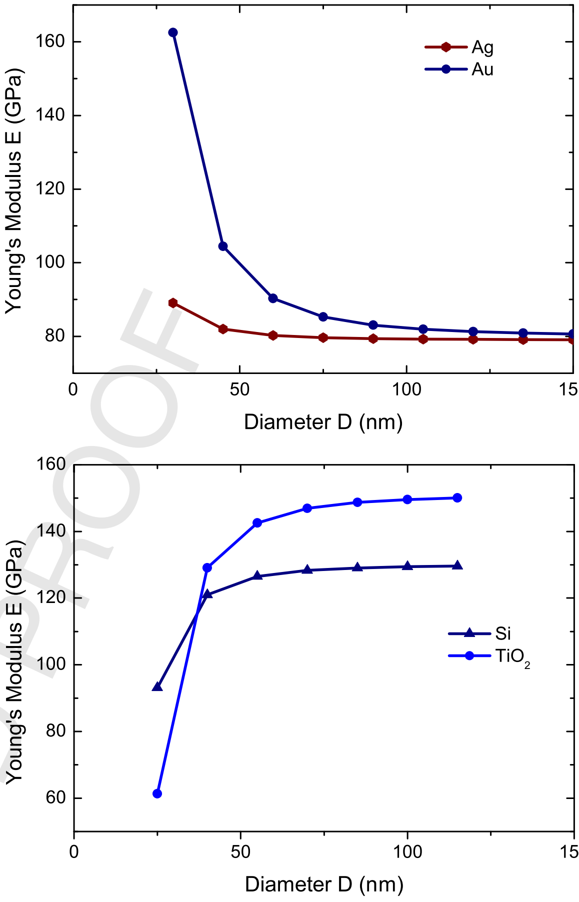

Fig. 1. Behavior of Young moduli as a function of diameter for relaxed metal and semiconductor NWs.

Also, we have shown the effect of diameter on the equilibrium strain (Fig. 3). Equilibrium strain increases with the decrease in diameter and is almost constant at larger diameters (at about 30 nm); in that stage the diameter reaches its bulk limit. As equilibrium strain is independent of surface stress, the behavior of strain as a function of diameter for both relaxed and unrelaxed metallic and semiconductor NWs was found to be the same. This is so, because the surface stress is the primary key for the change in the behavior of the Young modulus of the NWs, and also for the surface being relaxed or unrelaxed. This result is in good agreement with the previous studies [3,14] and also consistent with the experimental data available [3].

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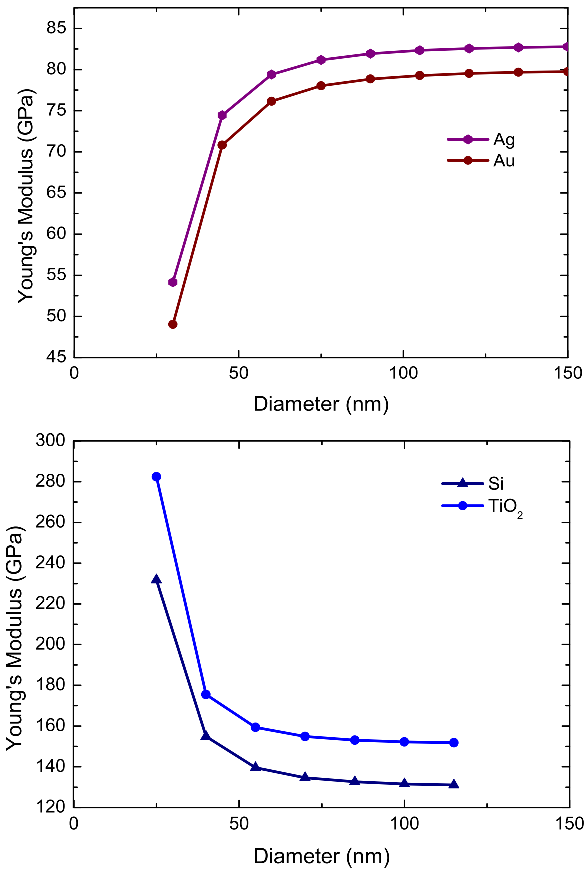

Fig. 2. Behavior of Young's moduli as a function of diameter for unrelaxed metal and semiconductor NWs.

3.2. DNA nanowires

We have taken into account fully relaxed DNA NWs, the torsional strain and the surface stress. As DNA possess a double helical structure, from previous calculations it can be seen that in a fully relaxed state, due to a torsional strain, surface stress in the DNA nanowires equals -0.6 J/m^2 [1]. As the surface stress is compressive (i.e. negative) we get to see a semiconductor-like behavior of DNA NWs Young modulus with diameter (Fig. 4): there is a significant decrease in the Young modulus of DNA NWs with decrease in diameter [1,14]. As the size of DNA NWs decreases, the number of atoms occupying the surface, which are more loosely bound than the bulk atoms, increases, which results in the decrease of Young modulus with decreasing diameter.

Unlike some of the semiconductor nanowires (ZnO) [4,14], DNA nanowires, although portraying semiconductor behavior, do not show a negative Young modulus marking their mechanical stability. Thus, we can conclude that beyond a certain diameter DNA nanowires do not show a phase transition.

An important role in determining the Young modulus of the NWs is played by the equilibrium strain. In Fig. 5 the effect of equilibrium strain on different sizes for relaxed DNA NWs is shown. The strain increases with the decrease in diameter and this result is somewhat different from the behavior of relaxed semiconductor NWs, where this increase is much sharper and at smaller diameters. This behavior marks its equivalent contribution, in contrast with that of surface stress, in determining the Young modulus of DNA NWs and it is due to the fact that Young modulus of DNA NWs decreases to a limit when it becomes smaller than the bulk modulus, giving an exponential increase in the equilibrium strain with decrease in the diameter [2].

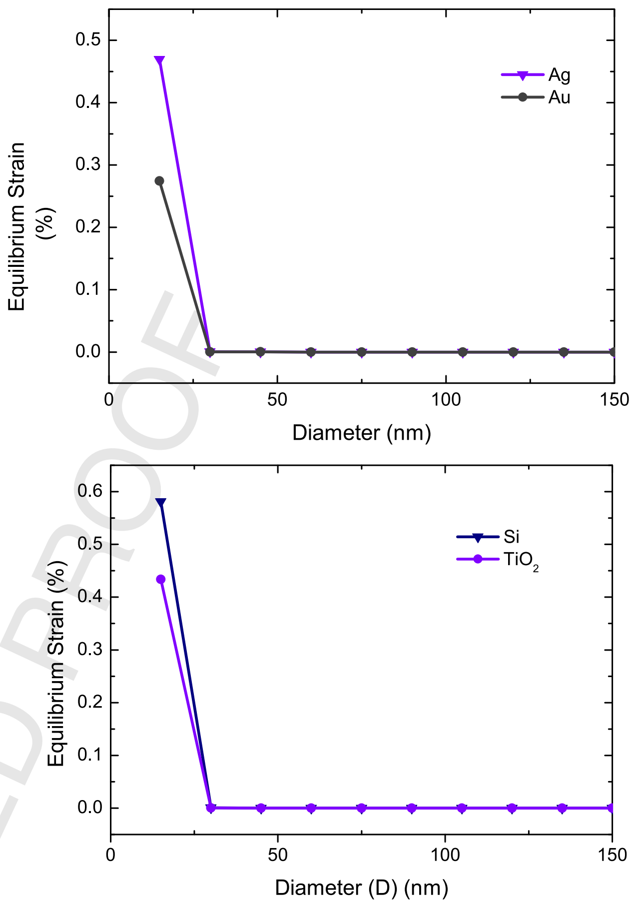

Fig. 3. Equilibrium strain as a function of diameter for metallic and semiconductor NWs, respectively.

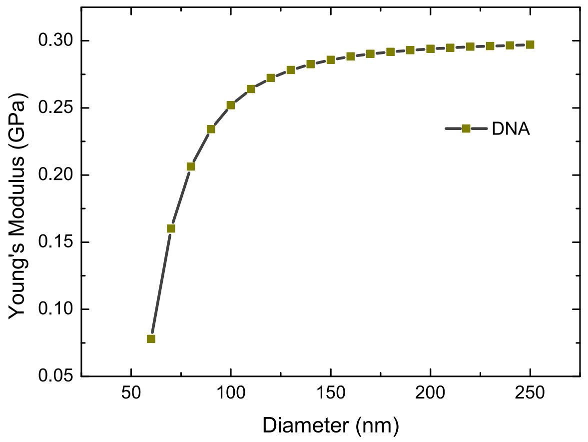

Fig. 4. Young modulus as a function of diameter for DNA NWs calculated for surface stress $g = -0.6$ J/m^2.

Intrestingly, a similarity of the nature of DNA NWs with that of the unrelaxed metallic NWs can also be seen. From Figs. 2 and 4, it is clear that the negative surface stress leads to the similarity between the two systems. Hence, a particular value is taken into consideration regarding the torsional strain and for this value for a fully relaxed DNA nanowire we get a semiconductor behavior.

From the above results it is clear that the key factors in determining the elastic properties and behavior of DNA NWs are surface stress, strain and the Poisson's ratio. Also, the diameter and surface stress play a pivotal role in estimating and understanding the behavior of the DNA NWs.

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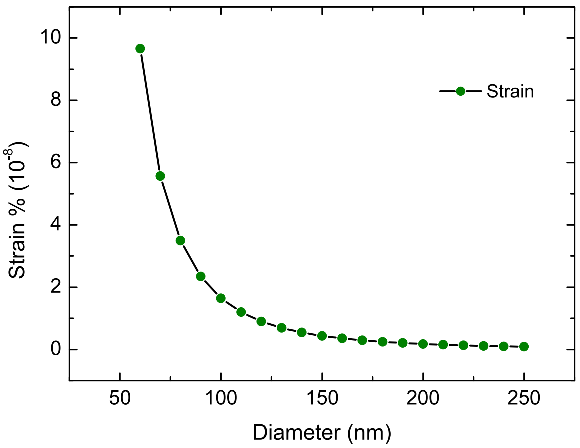

Fig. 5. Strain as a function of diameter for DNA NWs.

4. Conclusions

Our calculations suggest that coherence can be seen between the natures portrayed by relaxed semiconductor and unrelaxed metallic NWs with that of the DNA NWs. Due to this, it becomes very clear that this resemblance leads us to the conclusion that DNA NWs behave as a semiconductor at fully relaxed condition. This is also supported by the fact that the surface with positive (tensile) surface stress will lead to an increase in Young modulus whereas the surface with negative (compressive) surface stress will lead to a decrease in the Young modulus of the NWs with decreasing diameter. This may very well be the factor responsible for the different behavior of DNA nanowires regarding different surface stresses.

Thus, as the surface stress plays an important role we can see that it might be the possible key factor in engineering the desired mechanical properties. From our metallic and semiconductor investigations we have found that the surface stress plays an important role in determining the Young modulus of the nanowires and, along with contributions from equilibrium strain, responsible for the bi-conductivity of DNA NWs.

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References

[1] S. Cocco, J.F. Markob, R. Monasson, C. R. Phys. 3 (2002) 569–584.
[2] S. Dabhi, P.K. Jha, Adv. Sci. Eng. Med. 6 (5) (2014) 573.
[3] G. Wang, X. Li, J. Appl. Phys. 104 (2008) 113517.
[4] G. Wang, X.D. Li, Appl. Phys. Lett. 91 (2007) 231912.
[5] M. Lazzeri, A. Selloni, Phys. Rev. Lett. 87 (2001) 266105.
[6] L. Borgese, M. Gelfi, E. Bontempi, P. Goudeau, G. Geandier, D. Thiaudière, L.E. Depero, Surf. Coat. Technol. 206 (2012) 2459.
[7] N.W. Ashcroft, N.D. Mermin, Solid State Physics, Holt, Rinehart and Winston, New York, 1976.
[8] G. Simmons, H. Wang, Single Crystal Elastic Constants and Calculated Aggregate Properties: A Handbook, MIT, Cambridge, 1971.
[9] R.C. Cammarata, Prog. Surf. Sci. 46 (1994) 1.
[10] B. Wu, A. Heidelberg, J.J. Boland, Nat. Mater. 4 (2005) 525.
[11] G.Y. Jing, H.L. Duan, X.M. Sun, Z.S. Zhang, J. Xu, Y.D. Li, J.X. Wang, D.P. Yu, Phys. Rev. B 73 (2006) 235409.
[12] H. Ni, X.D. Li, Nanotechnology 17 (2006) 3591.
[13] R. Rudd, B. Lee, NSTI Nanotech 1 (2007) 524. Q2
[14] A. McEwan, S.K. Gupta, AIP Proc. (2015), in press.

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