ISSN NO. 2320-5407

Journal homepage: http://www.journalijar.com

INTERNATIONAL JOURNAL
OF ADVANCED RESEARCH

RESEARCH ARTICLE

Size dependent Young’s modulus of semiconductor nanowires: A theoretical approach

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Manuscript Info

Manuscript History:

Received: 14 October 2015
Final Accepted: 16 November 2015
Published Online: December 2015

Key words:

Nanowires, Semiconductor, Stress and Strain, Young’s Modulus.

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Abstract

The present paper reports the Young’s modulus of semiconductor (viz. ZnO and TiO_2) nanowires as a function of diameters considering both equilibrium strain and surface stress effect. A good agreement between the present calculated and available theoretical size dependent Young's modulus is found. The variation of relaxed/unrelaxed bulk materials surface and its effect on the Young’s modulus of the semiconductor nanowire is also demonstrated. A tensile (positive) surface stress can lead to an increase in the Young’s modulus and the decrease can be a result of a compressive (negative) surface stress. The surface stress plays an important role in determining the mechanical properties of the semiconductor nanowires.

INTRODUCTION

Nanowires (NW’s) are one of the most studied nanomaterials in recent years. A decent understanding of the size dependence of their Young’s modulus will further lead to make out their mechanical properties for the practical applications. Despite several previous studies dealing with the elastic properties of NWs, this issue requires an additional effort in order to systematically describe the dependence of the Young’s modulus with NW parameters such as size, shape and orientation etc. Usually, the diameter of semiconductor nanowires exert a great influence on its overall mechanical properties which is believed to be determined by the contribution of both bulk elastic modulus and surface elastic modulus. So, it is of great interest to explore how to estimate the Young’s modulus of the nanomaterials from their surface and strain effect. In the present work, we study the mechanical properties like Young’s modulus of semiconductor (viz. ZnO and TiO_2) nanowires of different sizes.

Theoretical Approach

In order to understand the Young’s modulus of the nanowire we have considered the effects of the two phenomenon like (1) effect due to equilibrium strain and (2) effect due to surface stress as discussed in the ref. [1] and can be written as,

$$E_{\mathrm{nanowire}} = (1+\epsilon^{*})^{2} + \frac{8}{5} g(1-v)\frac{L^{2}}{D^{3}} \qquad (1)$$

Where D is the diameter of the nanowire, L is the length of the nanowire, v is the Poisson’s ratio and ϵ^{*} is the equilibrium strain and g is the surface stress. As, the diameter of the nanowires increases, the equilibrium strain approaches to zero. Therefore, when D reaches the limit of bulk materials E_{nanowire} would be equal to the bulk modulus (E_b). Further, it is the elastic modulus of infinitely large extended surface, and ϵ^* is the strain at which the surface energy reaches its minimum. The physical parameter are used in the present work is listed in Table 1.

Results and Discussion

In the present paper, we present our results on the investigation of the Young’s modulus of semiconductor nanowires. Here, the length of the nanowire is assumed to be 1000 nm [1], the typical length suspended when the nanowire is suspended using three point’s clamped bending condition. Figure 1 shows a significant decrease in the Young’s modulus of the nanowire with the decrease in the diameter for both the nanowires with $D > 25\ nm$. This decrease of Young’s modulus of the nanowires is due to the surface stress effect [3]. The results are in good agreement with the theoretical predictions and also consistent with the experimental data [3-5]. The results shows a negative Young’s modulus of both of the nanowires with diameters less than 20 nm which may be due to their mechanical instability [3].

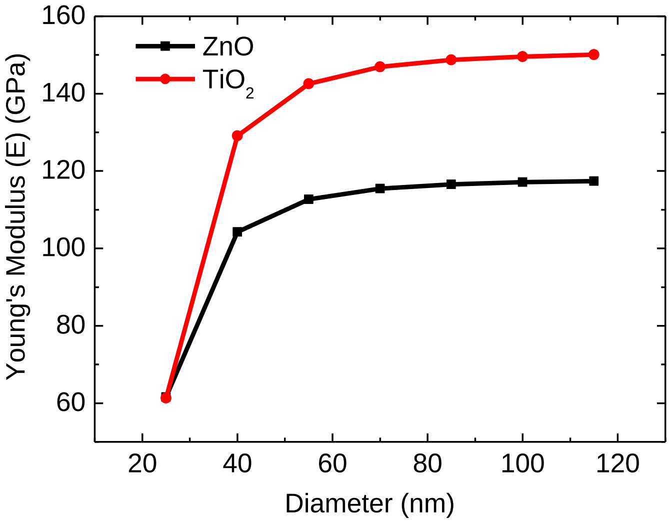

Figure 1. Young’s modulus vs. diameter for the semiconductor (viz. ZnO and TiO_2) nanowires calculated for relaxed surfaces.

This result is in agreement with the fact that ZnO nanowire below some critical size undergo phase transition from wurtzite to graphite crystal structures results higher Young’s modulus at decreasing diameters [3] due to change the surface stress. It is due to the fact that surface stress is negative for relaxed bulk materials. Therefore, figure (1) shows a decrease trend of Young’s modulus of the both nanowires.

Table 1: Physical parameters for both semiconductor (viz. ZnO and TiO_2) nanowires, where, a: relaxed and b: unrelaxed surfaces respectively.

system	Young’s modulus of Bulk Material E (GPa)	Poisson’s ratio (ν)	Surface stress in J/m^2
ZnO	118^a [3] 118^b [3]	0.32^a [3] 0.32^b [3]	-0.81^a [3] 1.3^b [1]
TiO_2	151^a [5] 151^b [5]	0.27^a [5] 0.27^b [5]	-1.2^a [4] 0.9^b [4]

While figure (2) shows an increase in the Young's modulus, for unrelaxed bulk materials which exert a positive surface stress [3]. For, both nanowires show a significant increase in the Young's modulus and this is due to the influence of the surface stress.

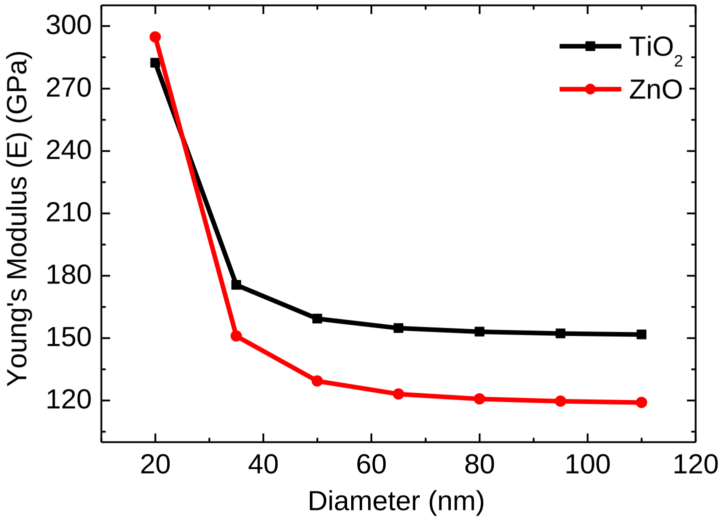

Figure 2. Young's modulus vs. diameter for semiconductor (viz. ZnO and TiO_2) nanowires calculated for unrelaxed surfaces.

The result is in good agreement with the theoretical results and we can see that till a certain diameter the increase is almost steady. This is because when D reaches its limit the Young's modulus equals the bulk modulus [1] as listed in Table 1. The equilibrium strain plays an important role in determining the Young's modulus of the nanowires. We have shown here only for relaxed surface, the strain effect on different sizes of semiconductor (viz. ZnO and TiO_2) nanowires as shown in figure (3). Figure reveals that the strain increases with the decrease in the diameter and this leads to the increase in the Young's modulus of the nanowires. This is due to the fact that as the size of the nanoparticles decreases, more number of atoms occupy surface, which are more loosely bound than the bulk atoms and responsible for the increase in the Young's modulus. It is also seen from the figure that below 20 nm size, the effect of strain is more significant leading to change in the mechanical properties.

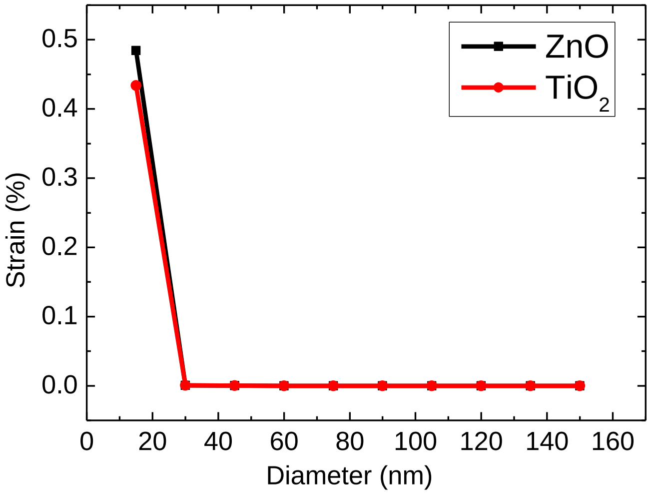

Figure 3. Strain vs. diameter semiconductor (viz. ZnO and TiO_2) nanowires calculated for relaxed surfaces.

Conclusion

The result suggests that the semiconductor nanowires can give different natures with the same diameter if the surface stresses are altered. We mainly focus on the variation that occurs when we consider a relaxed/unrelaxed surface and its effect on the Young's modulus of the nanowire. It is clear that a surface with positive (tensile) surface stress will lead to an increase in the Young's modulus whereas the surface with negative (compressive) surface stress will lead to a decrease in the Young's modulus of the nanowire and interestingly the curve seems to be exponential decay or rise. 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.

References

G. Wang and X. Li, J. Appl. Phys. 104, 113517 (2008).

S. Dabhi and P. K. Jha, Advanced Science, Engineering and Medicine 6(5), 573 (2014).

G. Wang and X. D. Li, Appl. Phys. Lett. 91, 231912 (2007).

M. Lazzeri and A. Selloni, Phys. Rev. Lett. 87, 266105 (2001).

L. Borgese, M. Gelfi, E. Bontempi, P. Goudeau, G. Geandier, D. Thiaudière, L.E. Depero, Surface & Coatings Technology 206, 2459 (2012).