



ISSN NO. 2320-5407

*Journal homepage: <http://www.journalijar.com>***INTERNATIONAL JOURNAL
OF ADVANCED RESEARCH****RESEARCH ARTICLE****Size Dependent Young's Modulus of Metallic Nanowires: A theoretical approach****Andrews McEwan and Sanjeev K. Gupta***

Department of Physics and Electronics, St. Xavier's College Ahmedabad, 380009, India.

Manuscript Info**Manuscript History:**

Received: 29 October 2014

Final Accepted: 26 November 2014

Published Online: December 2014

Key words:Nanowires, Metal, Stress and Strain,
Young's Modulus***Corresponding Author****Sanjeev K. Gupta****Abstract**

We have calculated the Young's modulus of nanowires as a function of nanowire diameters considering both equilibrium strain effect and surface stress effect, and carried out a simple theoretical approach to calculate the Young's modulus of metal nanowires viz. Ag, Au, Cu, Al, Ni, and a model adequate enough to predict. Consequently, we found that surface stress and the diameter plays a very important role in determining Young's modulus of nanowires.

*Copy Right, IJAR, 2014.. All rights reserved***Introduction**

Due to the possible applications in the scheme of technology and also in the commercial world such as nano electronics, photonics, biological and chemical sensors and resonators, metal nanowires without any qualm are of a great importance. A decent understanding of the size dependence of their Young's modulus will further lead to make out their mechanical properties for practical applications

Because of their reduced size, nanomaterials exhibit numerous challenges such as their measurement or manipulation of their physical properties. The intensive interest in nanowires is primarily due to their small size that recurrently leads us to exclusive physical properties which are not observed in their complementary bulk counterparts. Because of these unique properties the metallic nanowires have created symbolic interest in their use as the elementary building blocks of the future multifunctional nanoelectromechanical systems (NEMS) [12] that utilizes one-dimensional (1D) nanomaterial's as its effective components to initiate, transmit, and convert powers and motions [1].

This alterations in the diameter of the nanowires result in variance in the tensile and the elastic property of the metal nanowire. We study the Young's modulus of the nanowire in order to study the reliability and the strength of the nanowire. The mechanism of how Young's modulus of 1D nanomaterials depends on their size and surface conditions is shown in the present work. Usually, the diameter of these nanomaterials exerts 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 [4, 5, 6]. The relative alteration (i.e. increase or decrease) in the elastic properties of these nanomaterials may be as a result of the differing diameters, the surface bonding [7] and nonlinear bulk phenomena that are observed [8].

The experiments with the nanowires having cross-sectional sizes less than 20 nm [9, 10] agree with theoretical results [11] regarding the size dependence observed in metallic nanowires [12, 13]. In this paper, we have calculated Young's modulus of some metallic nanowires. Our model mainly focuses on the role of diameter in determining Young's modulus of metallic nanowires.

II. Theoretical and Numerical Approach

1. Young's Modulus of Nanowire

The total energy the nanowire can be expressed as a sum of the energy contributed from bulk and surface materials referring the previous studies as,

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

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

2. Effect of equilibrium strain

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

$$E_{\text{core}} = (1 + \varepsilon^*)^2 K_b \quad (2)$$

3. Effect of surface stress

We know that surface stress ($g = \gamma + d\gamma/d\varepsilon$) is the reversible work per unit area which is required to elastically stretch a surface [19]. We know that the 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. This results into 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's modulus of nanowires [13, 17, 18]. Hence, Young's modulus contributed from the nanowire's surface is given by,

$$E_{\text{surface}} = \frac{8}{5} g(1 - \nu) \frac{L^2}{D^3} \quad (3)$$

We know that the young's modulus of the nanowire is the sum of the core and the surface Young's Modulus given by the following equation as referred from the study. And it is given as,

$$E_{\text{nanowire}} = (1 + \varepsilon^*)^2 + \frac{8}{5} g(1 - \nu) \frac{L^2}{D^3} \quad (4)$$

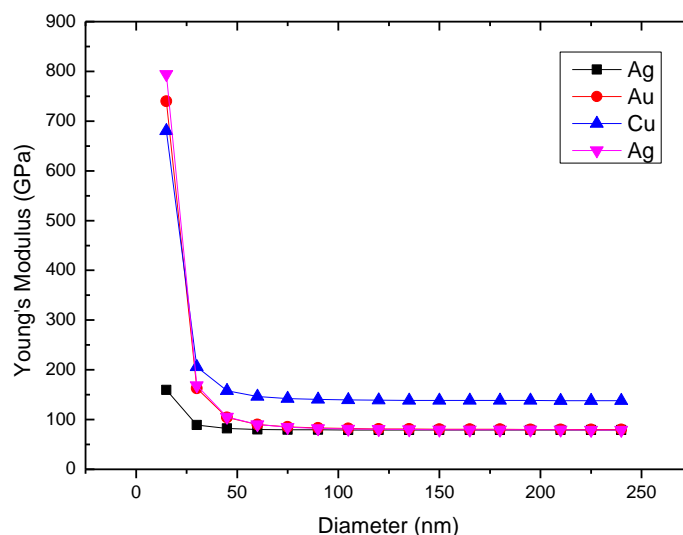
Where D is the diameter of the nanowire, ' L ' is the length of the nanowire, ' ν ' is the Poisson's ratio and ' ε^* ' is the equilibrium strain. As, the diameter of the nanowires increases, the equilibrium strain approaches to zero according to the above equation. Therefore, when D reaches the limit of bulk materials E_{nanowire} would be equal to the bulk modulus (E_b). Based on Eq. (3). in Fig. (1), we have plotted Young's modulus of the nanowires w.r.t the diameter to study the behavior of the nanowires and also to estimate their Young's moduli as a function of diameter.

RESULTS AND DISCUSSION

In order to examine the reliability of Eq. (3) we have calculated the Young's modulus of metal nanowires. Here the length of the nanowire is assumed to be 1000 nm, the length that is normally suspended when the nanowire is suspended using three point clamped bending condition [1]. To our approximation the results agree with the theoretical calculations and show nature as predicted by the calculations.

Graph of Enano vs. Diameter:

Fig (1), shows a significant decrease in the the young's modulus of the nanowire with the increase in the diameter. Intrestingly, this decrease of the various metal nanowires considerd seems to be exponential in nature [20]. But, the fact worth noticing is the drastic decrease in the Young's modulus at lower diameters which is followed by a steady decrease at higher diameters.



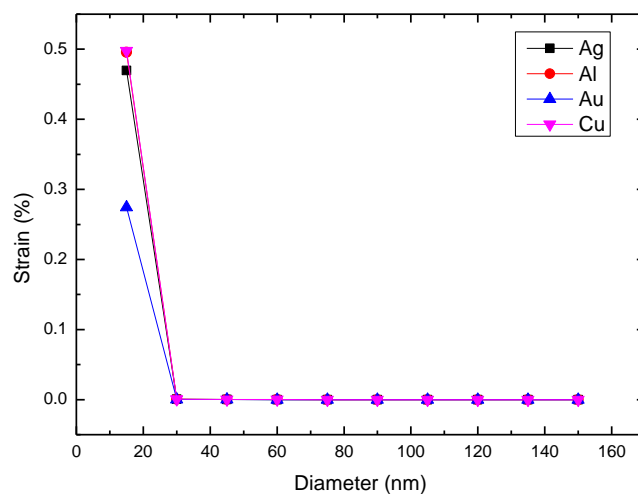
For, 100 nm diameter of the nanowire we can see that the decrease in the Young's modulus of all the metal nanowires almost shows the same behaviour, supporting the result that at higher diameters the Young's Modulus of the nanowires becomes almost same as the bulk modulus of their counter-parts as the diameter reaches it's bulk material limit.

Eventhough it was earlier believed that the Young's modulus of the Au NWs remained "independent" of diameter [1], studies show that the Young's modulus of the Au NW depend on diameter. Studies also show that that the decrease in young's modulus of the metallic NWs becomes slow when the NWs reach 75 nm mark and the increase reduces to 9% to that of the bulk modulus [1,17].

Graphs of Strain vs. Diameter:

We can also note that our obtained results are in agreement with the previous studies to a large extent. It is because from Fig. (2) we can see that the behavior of decrease in the strain regarding all the other specimens considered are almost identical and exhibit the same nature at higher diameters showing a steady decrease.

From the above results obtained we can figure out that the key factors that play an important role in determining the properties and the behaviour are none other than the surface stress, strain and the poissons ratio, except for the diameter which is deciding and the dependency factor in estimating and understanding the behaviour of the metal NWs.



CONCLUSION:

In this work, using the results and the conclusions from the previous studies; we have developed a model to estimate the Young's modulus of metallic NWs taking into consideration the properties of the corresponding surface and bulk counter-parts. Here, we have included two effects which are equilibrium strain and surface stress in our model to stand for the influence of the diameter on the elastic properties of these NWs based on the study that the Ag and Au NWs have a positive surface stress [1]. In order to precisely point out the effects due to surface stress, we focus on studying the effect of diameter on the Young's modulus with the help of clamped-end three-point bending loading condition [1, 13, 17, 18].

Furthermore, we calculated the Young's modulus of the NW with the help of the Eq. (3) derived in the theoretical analysis of the metal NWs. Considering, the inputs to be the theoretical data, and considering the Young's moduli of Ag, Au, Cu, Al, Ni NWs as functions of the equilibrium strain and NW diameter we have estimated the Young's moduli of the metal NWs.

Acknowledgements

We would like to thank the Principal Fr.(Dr.) Robert Arockiasammy, and Dr. Rajesh Iyer, HOD Department of Physics and Electronics, St. Xavier's college for providing with the opportunity and supporting for the same.

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