RESEARCH ARTICLE

MECHANICAL PROPERTIES OF RNA NANOWIRES

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Manuscript Info

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Abstract

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RNA is a polymeric genetic bio-molecule found in all human beings. It is the main genetic material in many viruses. In this paper we test the mechanical properties of RNA NWs. We will find Young's Modulus of RNA Nanowires (NWs) as a function of diameter with taking equilibrium strain, Poisson's ratio and surface stress in consideration. As previously no study has been published regarding Young's Modulus of RNA we take a theoretical approach towards it. We will predict the behavior of RNA NWs and see the resemblance to either semiconducting or metallic nature of NWs. This study extrapolates key factors in modelling RNA NWs for the creation of nanowires based aptasensors, genetics and other related applications.

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Introduction:-

Ribonucleic Acid (RNA) is a single stranded polymeric molecule essential for various biochemical roles in coding, decoding, regulation, and expression of genes. But in most organisms (except viruses mainly) RNA mainly acts as a messenger (mRNA) for the creation of specific proteins asked by DNA (deoxyribonucleic acid). It also acts as a structural component for ribosomes (rRNA) and as a coupler between two genetic codes and protein blocks (tRNA). RNA can be mainly of two types single stranded RNA (ssRNA) found in most organisms and double stranded RNA (dsRNA) found mainly in viruses.

Recently, RNA has been a topic of high interest for engineering nanowires as they have exceptional length control while being chemically robust makes them an effective template for formations of nanowires. Via bio-recognition-directed assembly method, its nanostructures can be assembled into functional devices. The interest in RNA nanowires exists because it is one of the key genetic material for both developed and under-developed organisms. Organisms like viruses have RNA as their main genetic material rather than DNA which is found in many developed organisms. Another reason is because of it being a really good candidate for nanowire based aptasensors. And different type of RNA especially dsRNA has a huge interest as a potential NW. And lastly, the interest exists in RNA NWs because of its elastic strain and charge potential. Due to this a few exclusive physical and mechanical properties are observed which are better in their complementary bulk counterparts.

Due to the diameter of these nanomaterials, the contribution of both surface elastic modulus and bulk elastic modulus is believed to have a great influence over all mechanical properties. Maybe as a result of differing diameters, the surface bonding and observed nonlinear bulk phenomenon, the relative increase or decrease in the elastic properties is seen. Having the same order of magnitude as Au (gold) NWs, an analogy for elastic vibrations these RNA NWs can be set. The typical RNA NWs are minuscule pockets of proteins and are well known as genetic

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material. So, it is both now an interesting and an important topic to explore and study the Young's modulus regarding their bulk material and surface properties.

In the current work, we mainly focus on mechanical properties of RNA NWs, like Young's modulus along with relaxed/unrelaxed metal and semiconductor NWs. Also, we gain insight into the similarities of different properties of RNA NWs, which helps us efficiently predict the nature and applications of RNA NWs. Therefore, the application of NWs in various fields of nano-science can be increased as nanowires can be synthesized by taking an account of their properties and effects of diameter on their properties.

Materials and Methods:-
The total energy of a nanowire can be represented as sum of energy contributed from surface and bulk materials

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

Here, $\Omega(\varepsilon)$ is the bulk energy density in the nanowire core $\gamma(\varepsilon)$ is the surface energy of nanowire, D is diameter of nanowire, L is the length of nanowire.
Now, let δ be a strain by which the nanowire is deformed from its equilibrium state due to some load (where ϵ^* is the equilibrium strain). Then, $\delta = \frac{\epsilon}{(1+\epsilon^*)}$
(Here ϵ is the strain in accordance with the equilibrium strain). Hence, Young Modulus contributed from the nanowire's core should be

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

Here, E_s is the surface elastic modulus whereas E_b is the bulk elastic modulus. We know that surface stress ($g = \gamma + \frac{d\gamma}{d\varepsilon}$) is reversible work per unit area required to elastically stretch a surface. The total surface area changes by $\pi D(1 - \nu)\Delta L$ (ν is Poisson's ratio) when a circular nanowire is subject to deformation. This causes change in energy which is associated with surface deformation of 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 clamp-end three-point bending, which is most often used to measure Young's Modulus of NWs. Hence, the surface stress is

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

Also, we know that in a nanowire, the Young's Modulus in terms of surface stress and diameter is sum of core and surface Young's Modulus, hence from above equation,

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

Therefore, we can see that with increase of diameter, the equilibrium strain tends to zero according to equation (3). Hence when diameter reaches the limit of bulk materials $E_{nanowire}$ would be equal to the bulk modulus (E_b). Consequently, it is elastic modulus of an infinitely large extended surface, and ϵ^* is the strain at which surface energy reaches its minimum.

Table 1:- Values of Young's Modulus, Poison Ratio, and surface stress of different material.

System	Young Modulus E (GPa)	Poisson's Ratio (ν)	Surface Stress (J/m^2)
Ag	79[a]/79[b]	0.37[a]/37[b]	0.27[a]/(-0.773)[b]
Au	80[a]/80[b]	0.42[a]/0.42[b]	2.4[a]/(-0.901)[b]
TiO$_2$	151[a]/151[b]	0.27[a]/0.27[b]	(-1.2)[a]/0.9[b]
Si	130[a]/130[b]	0.29[a]/0.29[b]	(-0.5)[a]/1.38[b]
DNA	0.3[a]	0.5[a]	(-0.6)[a]
RNA	----	0.45[a]	0.038[a]

Results and Discussion:-

In our study we assumed the length of nanowire to be 1000nm, i.e. the typical length of nanowire when suspended using a three-point clamped bending. Hence, our results are based on the behavior of the Young's modulus of RNA NWs. Here, we will discuss RNA NWs behavior with constant diameter, also comparing its resemblance with either metallic or semiconducting behavior of NW.

Metallic and Semiconductor Nanowire

In order to understand behavior of RNA NWs we have to theoretically estimate the behaviour of metallic and semiconductor NWs in both relaxed and unrelaxed state. Also, we know that Young's modulus of metallic NWs for relaxed state is inversely proportional to diameter and for semiconducting NWs in relaxed state is directly proportional. This behavior is seen because the nature of surface stress. As it has been observed that the surface stress of relaxed metallic NWs is tensile (positive), whereas for semiconductors its compressive (negative). But for unrelaxed NWs the surface stress for metallic NWs becomes compressive while for semiconducting it becomes tensile.

RNA Nanowires

We have considered a fully relaxed RNA NW. As it is a single stranded structure its surface stress is ($+0.038$ J/m^2) tensile. Therefore, we get to see metallic NWs like behaviour of RNA NWs' Young's modulus. Also the Young's modulus can have a significant increase as diameter decreases because it exhibits traits similar to that of metallic NWs. And, interestingly they also have behaviour similar to unrelaxed semiconductor NWs. It is clearly observed that surface stress leads to a similarity between two systems, hence a particular value is required to establish a trend. All the factors, stress, strain Poisson ratio and diameter all play a pivotal role in estimating and determining the behaviour of RNA nanowire.
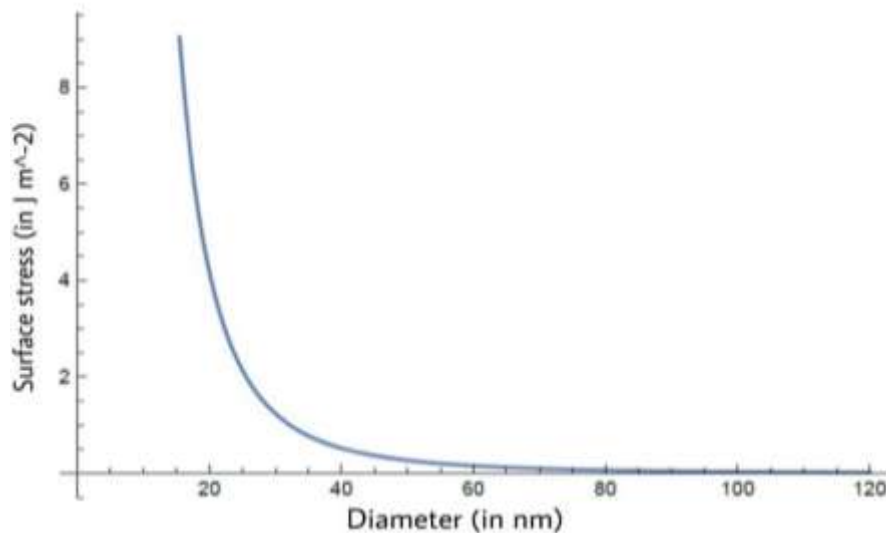

Figure 1:- Surface Stress and Diameter trend graph.

Conclusion:-

As we can see a coherence between RNA NWs and that of relaxed metallic NWs and unrelaxed semiconducting NWs. It is very clear that RNA NWs acts like metallic NWs at relaxed state and semiconducting NWs at unrelaxed state. This can also be proven with the fact that a nanowire with positive surface stress will lead to increase in Young's Modulus with decrease in diameter, and a body with negative surface stress will see a decrease in Young's Modulus with decrease in diameter of nanowire. This could be a reason for different behaviour of RNA NWs regarding different stresses. Hence, surface stress might play a key role in engineering the RNA NWs with desired mechanical properties. From our metallic and semiconductor behaviour investigations we found that surface stress plays an important role in determining the Young's Modulus of NWs along with equilibrium strain both of which leads to bi-conductivity of RNA NWs and establishing a trend between metallic and semiconducting nanoconductors.

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