



RESEARCH ARTICLE

EFFECT OF DIVALENT DOPING ON YOUNG'S MODULUS OF ZNO NANOWIRES.

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Abstract

The present work brings to light the effect of divalent (viz. Mg) doping on the Young's Modulus (YM) of ZnO nanowires (NWs), as a function of diameters considering surface stress effect. It is seen that the YM exhibits contrasting behavior for different doping concentrations of Mg. The variation in the YM is seen to be of semiconductive type, which then is seen to change to depict conductive type behavior on the immersion of Mg as a dopant. The doping along with surface stress play as deciding factors in determining the mechanical properties; especially the YM of the ZnO nanowires.

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Introduction:-

Thin Films and Nanowires are emerging as one of the most enticing fragments offered by the recent developments in the field of Nanotechnology in current times. Also, along with the Thin Films and NWs developed from pure undoped materials, a new horizon has been put forth by the concept of doping and the variation that this doping can bring in the material. More recent studies show that this idea of doping has proved to be an extremely valuable aspect as it can be used to unlock the hidden potentials and frontiers that the material has to offer. So, decent understanding of the outcomes of doping on semiconductor materials is essential. ZnO is one of the most commonly used semiconductor materials with a direct bandgap of ~3.37 eV at room temperature which leads to its abundant applications in the field of Photonics and Optoelectronics [1-4]. Previous Studies [5-7] of size dependence of YM of ZnO NWs has further lead us to explore out their mechanical properties for the practical applications. Along with diameter, the concentration of doping usually exerts a great influence on its overall mechanical properties; especially the YM 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 the YM of the ZnO NWs varies as a function of their diameters and concentrations of doping.

Theoretical Approach:-

In order to estimate the YM of the ZnO nanowires the effects due to surface stress as discussed in the ref. [5,6] and can be written as,

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

Where D is the diameter of the nanowire, L is the length of the nanowire, ν is the Poisson's ratio and g is the surface stress [5,6,10]. As, the diameter of the nanowires increases, the equilibrium strain approaches to zero [5,7]. Further,

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it is the surface stress that plays as an important parameter and changes with the change in the concentration of doping [5,6,9].

Results and Discussion:-

In this work, we bring forth our results on the investigation of the YM of Mg doped ZnO nanowires. Here, the length of the nanowire is assumed to be 1000 nm [5,6], the typical length suspended when the nanowire is suspended using three point's clamped bending condition. The concentrations of Mg doping in ZnO is taken to be 0%, 2%, 4%, 6%, 8% and 10%. We have seen that the ZnO shows different behavior for undoped (i.e. 0%) and the doped case (i.e. 0%, 2%, 4%, 6%, 8% and 10%. respectively) [9]. We have taken into consideration (100) and (101) directions of growth of the NWs at growth temperature and annealed at 500°C and 700°C with the data acquired from other studies regarding the same [9]. From Fig 1, we can see that the YM increases for the as grown state of the Mg doped ZnO NWs but we see that when we anneal the same at temperatures above 450°C, the YM decreases with decreasing diameters showing semiconductive behavior [5-7]. Previous studies [10] suggest that the crystallization in ZnO occurs after crossing the 300°C temperature which is believed to be one of the reasons that the following trends and behavior are seen in the undoped ZnO case. Also, it is seen that the increase in temperature of annealing leads to further decrease in the YM of undoped ZnO NWs.

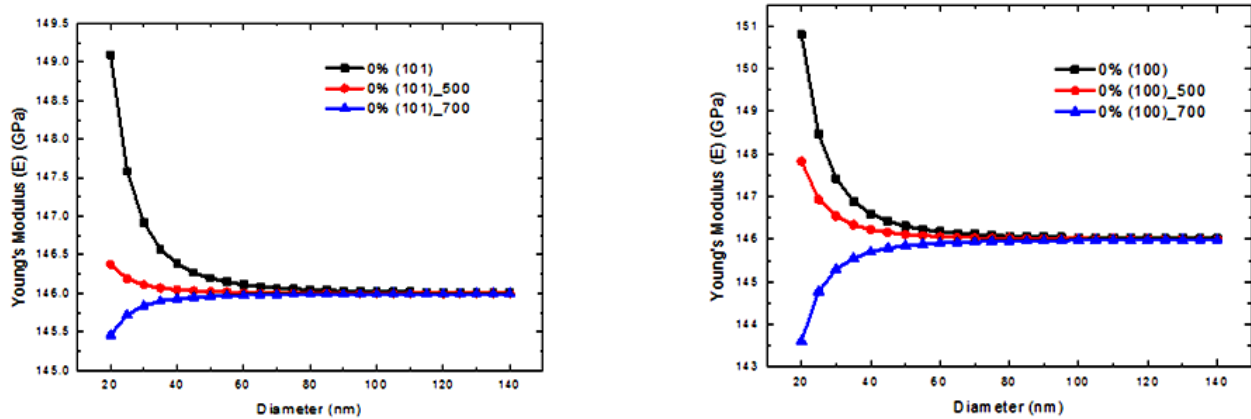


Figure 1:- YM vs. diameter for undoped ZnO NWs for (100) and (101) orientations at different temperatures.

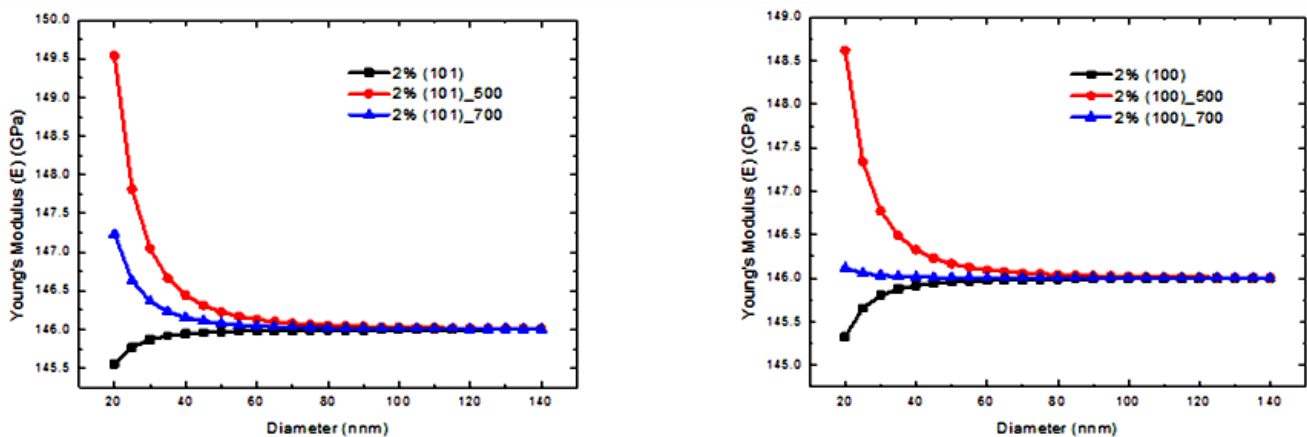


Figure 2:- YM vs. diameter for 2% Mg doped ZnO NWs for (100) and (101) orientations at different temperatures.

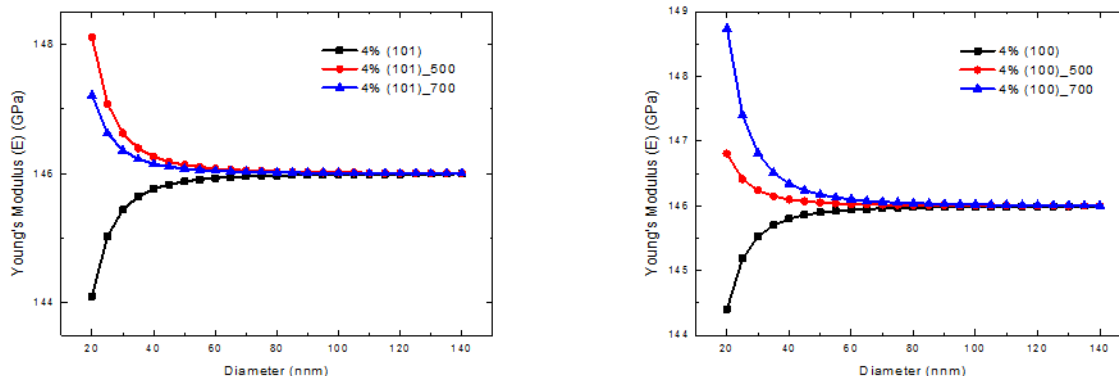


Figure 3:- YM vs. diameter for 4% Mg doped ZnO NWs for (100) and (101) orientations at different temperatures.

A similar approach was used to demonstrate the effect of Mg doping on the ZnO nanowires and it was observed that the results are quite exciting. It was seen that unlike the undoped case, the doping of Mg in various concentrations lead to an increase in the YM of the Mg doped ZnO NWs. The YM is found to increase with the decreasing diameters and hence show the conducting behavior [5] which is supported by the fact that the doping of Mg in ZnO leads to a change in bandgap of the material. Fig 2-6, show the effect of various doping concentrations on the YM of the ZnO NWs. An evident point is seen that as the doping concentrations increase the maximum value of YM of the NWs decreases. It may be because the effect of Mg doping on ZnO is substitutional. The peak value of YM in both orientations of growth is seen at 500°C for 2% doping and at 700°C for 4% doping of Mg showing the effect of doping on the crystallization temperature of the resultant material.

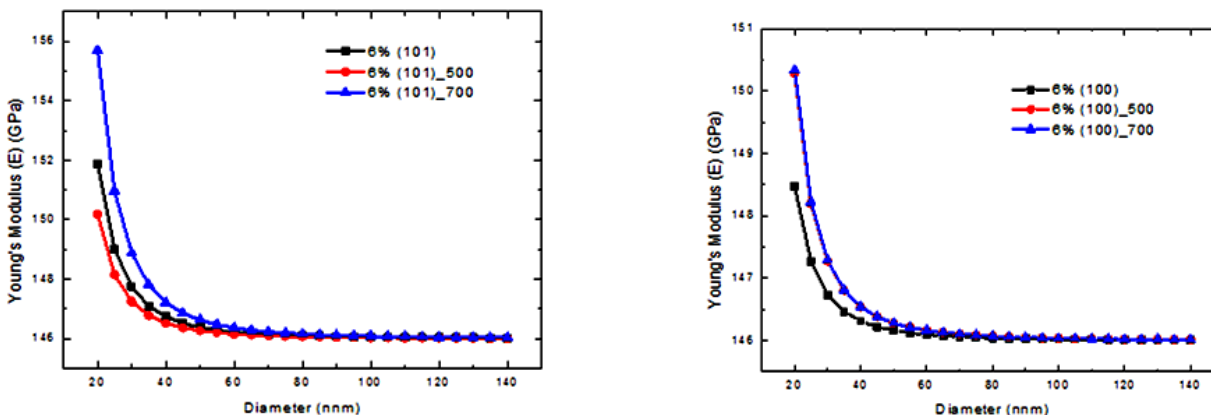


Figure 4:- YM vs. diameter for 6% Mg doped ZnO NWs for (100) and (101) orientations at different temperatures.

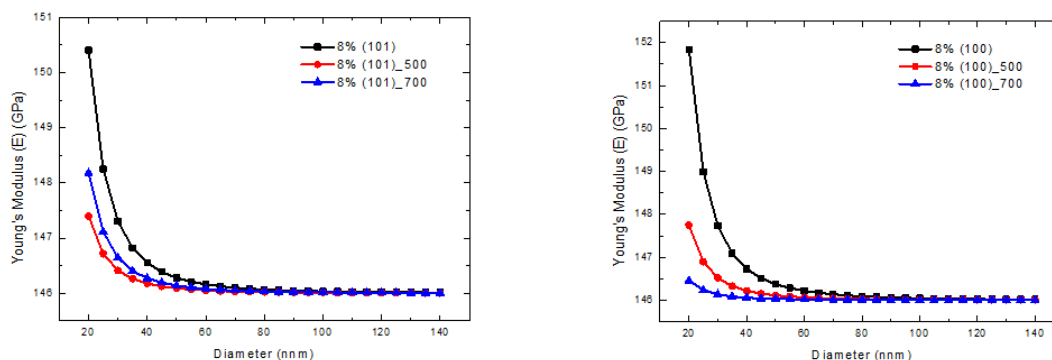


Figure 5:- YM vs. diameter for 8% Mg doped ZnO NWs for (100) and (101) orientations at different temperatures.

A major change in the behavior of the YM is seen from Fig. 4 and 5. It is seen that the trend of the YM for the as grown temperature is changed from the behavior exhibited in the previous two doping concentrations. The maximum value of YM for the 6% doping case was found to be at 600°C temperature which is in good agreement with the 4% result. But, to our surprise the maximum value of the YM unlike the above two cases was seen to be that of the sample at the growth temperature for both the orientations. This has opened a new window for us to explore as to how the above change has taken place.

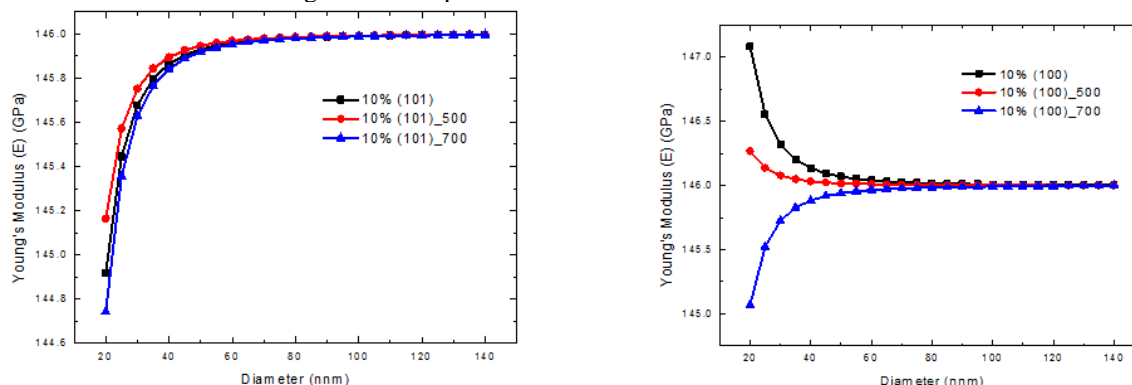


Figure 6:- YM vs. diameter for 10% Mg doped ZnO NWs for (100) and (101) orientations at different temperatures.

An even unexpected turn of behavior was seen in the 10% doping sample because it shows a decrease in the YM of the NWs with decreasing diameters in all the three temperatures at the (101) orientation, but at (100) orientation the behavior was seen to strike an unusual resemblance to that of the undoped case. This is yet to be seen as to what is the reason behind such a behavior seen in the NWs. All of the above discussed results have been computed from the values of the surface stress obtained from ref. 9 and we can see that the surface stress plays the deciding factor in the considered model for the estimation of behavior of Mg doped ZnO NWs. The variation in the surface stress with the corresponding change in the doping concentration of the material is shown in Fig7. This change in the surface stress is one of the pivotal reasons to the behavior observed in 8% and 10% doped samples.

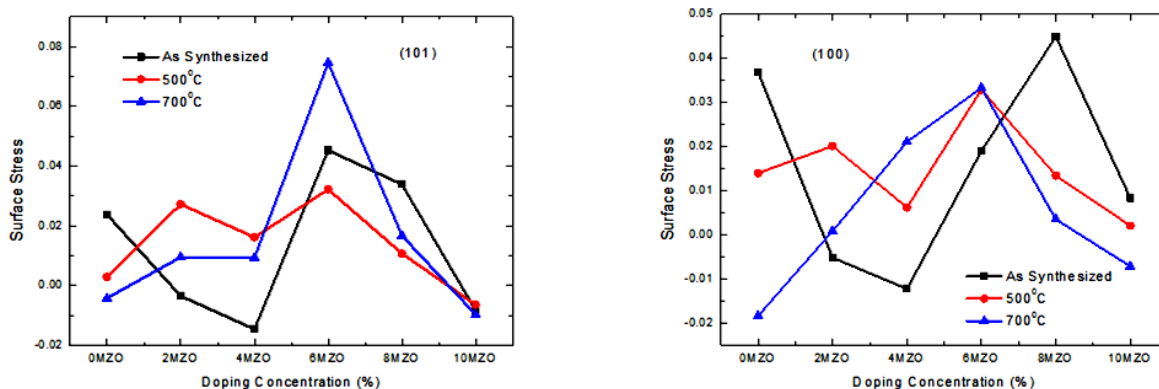


Figure 7:- Surface Stress vs. Doping Concentrations of Mg doped ZnO NWs for (100) and (101) orientations.

Conclusion:-

The results suggest that ZnO NWs can give different natures with the same diameter if the concentrations of doping are altered which would result in the respective change in the surface stress as well. We have mainly focused on the variation that occurs when we consider doping at different temperatures and orientations, and its effect on the YM of the NWs. It is clear that a surface with positive (tensile) surface stress will lead to an increase in the YM whereas the surface with negative (compressive) surface stress will lead to a decrease in the YM of the NWs[5-7]. 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.

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