



Effect of size and shape on young modulus of metallic nanosolid

ABSTRACT

The size and shape dependence of mechanical property of metallic (Ag and Au) nanoparticle, nanowire and nanofilm have been studied using a simple theoretical approach. There is an increase of the ratio of the Young's modulus at nanoscale to the bulk as size decreases. A good agreement between the present calculated and available theoretical and simulation size dependent Young's modulus is found. Present model is also useful for different shape of nanoparticle, nanowire and nanofilm.

Keywords: young's modulus, nanoparticle, nanowire, nanofilm, nanosolids, Ag, Au.

INTRODUCTION

Nanomaterials shows changed physical, thermal, optical, chemical and mechanical properties from the corresponding bulk materials, such as depression of melting temperature and thermal conductivity, increase in band gap of semiconductor, decreasing in dielectric constant and refractive index. Young modulus either increase or decreases depends upon the surface is relaxed or not. [1] These peculiar properties bring potential and broad application in microelectronics, optics, sensors and so forth. While elastic characterization of nanomaterials determines the stability and the reliability of the devices. Therefore to understand the size effect of elastic properties and their theoretical mechanism is important. The theoretical explanations for the size effect of the elastic modulus are related with the surface effect by introducing the surface energy contribution in the continuum mechanics [2] or by the computational simulations reflecting the surface stress [3,4] or surface relaxation influence[5,6].

Nanomaterials have changed Thermal and mechanical properties from the corresponding bulk materials due to increased surface to volume ratio and optical and electric properties due to increased quantum mechanical confinement.

In this paper we have developed simple model for predicting young modulus of metallic nanosolids using the concept of increased surface to volume ratio. Our predictions are in good agreement with available experimental data. It shows the validity of our work.

METHOD OF ANALYSIS

Total number of atoms in nanosolid are given by

$$n = N_i + N_s \quad (1)$$

Where N_i is the number of atoms inside nanomaterial and N_s is the number of atoms on the surface of nanomaterial.

$$N_i = n - N_s \quad (2)$$

$$N_i = n \left(1 - \frac{N_s}{n} \right) \quad (3)$$

Surface atoms have half contribution so the fraction of atoms inside the nanosolids

$$\frac{N_i}{n} = \left(1 - \frac{N_s}{2n} \right) \quad (4)$$

As the particle size decrease number of atoms inside the nanosolid decrease and atoms on the surface increases. so the fraction of the surface atoms is given by

$$1 - \frac{N_i}{n} = 1 - \left(1 - \frac{N_s}{2n} \right) \quad (5)$$

Since the tensile strength of material depends on the number of atoms on the surface if we introduce shape factor α , [7,8] for metallic nano solids equation (5) becomes

$$\frac{y_n}{y_b} = 1 + \left(1 - \left(1 - \frac{\alpha N_s}{2n} \right) \right) \quad (6)$$

OR

$$\frac{y_n}{y_b} = 1 - \left(1 - \left(1 - \frac{\alpha N_s}{2n} \right) \right) \quad (7)$$

Equation (6) is for relaxed surfaces and Equation (7) is for non-relaxed surfaces.

Here α is dimensional less shape factor. For nanoparticle [7] which is defined by the ratio of area of nanoparticle in any shape whose volume is the same as spherical nano particle to the area of spherical nanoparticle. For nanowire it is defined by the ratio of surface area of nanowire with arbitrary cross-sectional shape whose volume is same as cylindrical nanowire to the surface area of cylindrical nanowire.[8]

RESULT AND DISCUSSION

Input parameters required for computation are compiled in Table 1 and Table 2.

Table 1: Input parameters.

Element	Atomic diameter d(nm)
Ag	0.330
Au	0.348

Table 2: Computed values of N_s/n for different solids.

Nanosolids	N_s/n
Spherical nanosolid	$4d/D$
Nanowire	$(8/3)d/D$
Nanofilm	$(4/3)d/h$

Where d is diameter of atom and D is diameter of nanoparticle / diameter of nanowire and h is thickness of nanofilm.

Table 3: The calculated shape factor for different particle shape and for prism like nanowire with different cross-section

Particle shape	Shape factor (α)
Spherical	1
Regular tetrahedral	1.49
Regular hexahedral	1.24
Regular octahedral	1.18
Disc-like	>1.15
Regular quadrangular	>1.24
Prism- like nanowires with regular triangular cross-section	1.286
Prism- like nanowires with regular tetragonal cross-section	1.128
Prism- like nanowires with regular hexagonal cross-section	1.050
Nanowire with rectangular cross-section	1.13

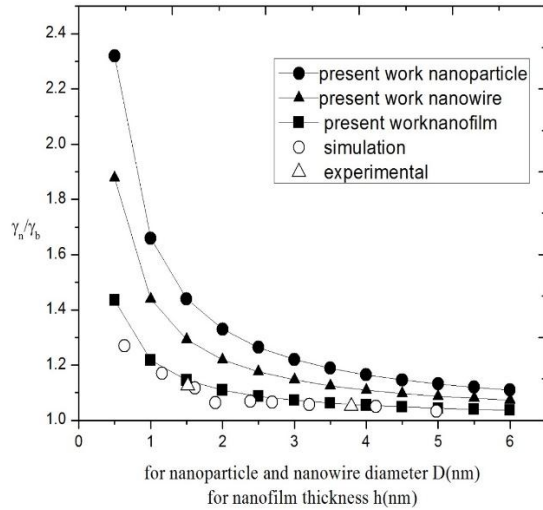


Figure 1: Ratio of Size dependent young modulus of nanosolids to bulk for Ag computed using equation (6)

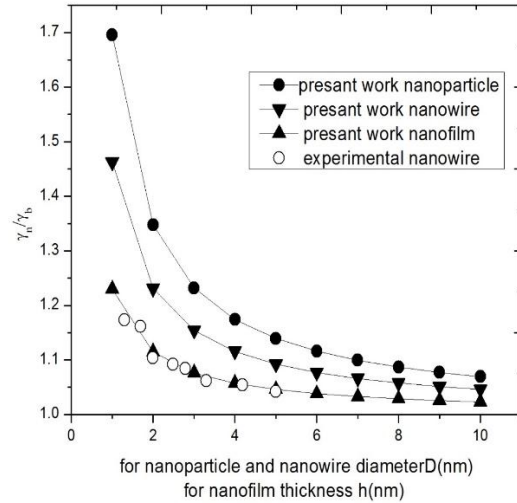


Figure 2: Ratio of Size dependent young modulus of nanosolids to bulk for Au computed using equation (6)

Results for the ratio of γ_n/γ_b for Ag nanoparticle, nanowire and nanofilm computed using eq.6 are compared with simulation [4] and experimental [9] evidences in Fig.1. It is found that the size dependent ratio γ_n/γ_b increases as the diameter of nanoparticle D decreases. Our results are in good agreement with experimental and simulation data

Results for the ratio of γ_n/γ_b for Au nanoparticle, nanowire and nanofilm computed using eq.6 are compared with experimental [10] evidences in Fig.2. It is found that the size dependent ratio γ_n/γ_b increases as the diameter of nanoparticle D decreases. Our computed results are slightly higher than experimental data of nanowire.

CONCLUSION

As the size of nanosolids decreases surface to volume ratio increase so number of atoms on the surface increases. Surface to volume ratio becomes more for smaller nanosolids. Due to increase in the number of atoms on the surface inter atomic distance decreases so interatomic force increase so shearing strength of nanomaterial increases so the young modulus of nanosolids increases. In conclusion we can say that the as diameter of nanoparticle and nanowire and thickness of nanofilm decreases young modulus increases. Our predictions are well agreed with available experimental and simulation data for Ag nanofilm. It gives the validity to our model. Our computation is for only for relaxed surfaces.

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