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# Prediction of elastic moduli of metallic nanoparticles

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**Abstract**
Predictions for the variation of physical properties of nanomaterials have been a matter of great debate in the recent decades. Different researchers have reported drastic change in the physical properties of metals at their nano scale. In the present work, we have studied the theoretical value ofYoung's modulus and Bulk Modulus of spherical nanosolid, nanowire and nanofilms of Aluminium (Al), Copper (Cu), Paladium (Pd) and Platinum (Pt) having their sizes less than 30 nm. For computation we have consider the fundamental relation of cohesive energy with melting point. During our study it is found that there is a drastic change in the elastic constants of spherical nanosolid, nanowire and nanofilms of metals below 20 nm. In this variation,it is also observed that there is maximum variation of elastic constants are in case of nanofilms while minimum in case of spherical nanosolids and moderate change in case of nanowires. Variation in elastic constants has been interpreted on the basis of the presence of number of surface atoms due to the change in surface to volume ratio of metals at the nano level.
**Key words:**Metallic nanoparticles, Elastic constants and Metallic nanostructure materials.

**Introduction:**
In the nanoscience and nanotechnology, the size of materials has reduced at the very low scale nanometer at least one dimension. In this size range, the surface to volume ratio is much increased and correspondingly the physical, chemical, and mechanical properties are changed [1-3]. The properties of material at nanoscale are different from the corresponding bulk material. The properties of nanomaterials change drastically as the size reduces below 30 nanometers. A sample of gold appears red at 10 nanometers. Its melting temperature decreases rapidly as their sizesare reduced up to the level of nano scale [4-5].
Our purpose is to determine the elastic constants of the nanomaterials which is closely related to the cohesive energy of the nanomaterials. The cohesive energy or heat of sublimation is an important physical quantity to account for the strength of metallic bonds. The cohesive energy is the energy to divide the metallic crystal into individual atoms. For the above said purpose we studied the equation of state for the size dependent elastic constants of the nanoparticles of metals Aluminium (Al), Copper (Cu), Paladium (Pd) and Platinum (Pt). We have computed the elastic constants of spherical nanosolid, nanowire and nanofilm of the considered samples. With the different mode of variation, it is observed that the elastic constants of metals at nano levelincreases with increase of theirsizes.

**Method of Analysis** :
The total cohesive energy of the nano crystalline solid, is given by

$$E_{tot} = E_0(n-N) + \frac{1}{2}E_o N \qquad \ldots(1)$$

Equation (1) is the sum of energy due to the contribution of the interior atoms as well as the surface atoms of nanocrystalline solids. Here $E_0$ is the cohesive energy of the bulk materials per atom, $n$ is the total no of atoms of nanosolid and $N$ is the number of atoms at surface. [6]
For the cohesive energy per mole, the equation (1) may be written as

$$A_v E_{tot} = E_0 A_v\,(n-N) + \frac{1}{2}A_v E_o N$$

$$\frac{A_v E_{tot}}{n} = E_0 A_v\left(1-\frac{N}{n}\right) + \frac{A_v E_0\, N}{2n} \ldots (2)$$

Where,$A_v$ is Avagadro number. The term $\frac{A_v E_{tot}}{n} = E_n$represents the cohesive energy per mole of the nanocrystalline solid and $E_0 A_v = E_b$ is the cohesive energy per mole of the corresponding bulk material.
Thus equation (2) becomes,

$$E_n = E_b(1-\frac{N}{2n}) \ldots (3)$$

Since the cohesive energy is linearly related to the melting temperature,[7-8], therefore the melting temperature of the nanosolid can be written as

$$T_{mn} = T_{mb}\,(1-\frac{N}{2n}) \ldots (4)$$

Also, the elastic moduli increase with increase in cohesive energy. Thus taking analogy of equation (3), we may write,

$$Y_n = Y_b(1-\frac{N}{2n}) \qquad \ldots(5)$$

And, $B_n = B_b(1-\frac{N}{2n}) \qquad \ldots(6)$

Here Y's and B's represent the Young's modulus and bulk modulus of material respectively.

The value of $\left(\frac{N}{2n}\right)$ depends upon the structure of the nanomaterial and has been calculated for different shape of nanomaterials [9].

For spherical nanosolids, $\frac{N}{2n} = \frac{2d}{D}$ …….(7)

Where, D and dare the diameters of spherical nanosolid and that for atom respectively.

For nanowires, $\frac{N}{2n} = \frac{4d}{3L}$ …….(8)

Where, L is diameter of nanowire.

And for nanofilm, $\frac{N}{2n} = \frac{2d}{3h}$ …….(9)

Where h is height of nanofilm.

**Table: 1:** Input Parameters of Eq.(5) and Eq.(6)

| Metals | Atomic Diameter,d(nm) .[10] |
|---|---|
| Copper (Cu) | 0.2822 |
| Palladium (Pd) | 0.3040 |
| Platinum(Pt) | 0.3064 |
| Aluminum (Al) | 0.3165 |

**Result and Discussion**

In our present work we have studied theoretically the variation of Young's modulus and bulk modulus of nanocrystalline metals given in the table-1. To compute the Young's modulus and bulk modulus of nanocrystalline copper, palladium, platinum and aluminum equation (5) and (6)are used in which the required input data has been taken from table-1 [10]. The computed values of Young's modulusof Cu, Pd, Pt and Al (nanosolid, nanowire and nanofilm) are plotted against the size of corresponding nanostructures, given in Fig.(1) – Fig.(4).During our study of size dependence of Young's modulus and bulk modulus, it is found that Young's modulus and bulk modulus of metal nanostructures decreases in the small range of their sizes (10-20nm) after that it becomes almost constant. The curves can be divided into two parts, sizes larger than 10 nm and sizes less than 10 nm. Elastic moduli change gently with the variation of size and the curves are nearly horizontal for D >10 nm. But the change in Elastic moduli is much rapid below 10 nmin case of these metallic nanostructuredmaterials. Again we can see that beyond 20 nm of the size of the material, the ratio of Elastic moduli at nanoscale to the bulk becomes almost constant. The universal relation for size dependent thermodynamic properties of metallic nanoparticles suggested by Xiong et al [11] also predict the same size dependent variation of melting point in case of metals.Also the change in Elastic moduli for nanosolids is larger than that of nanowires and nanofilms. This is due to the rapid increase in surface to volume ratio at smaller nanoscale.

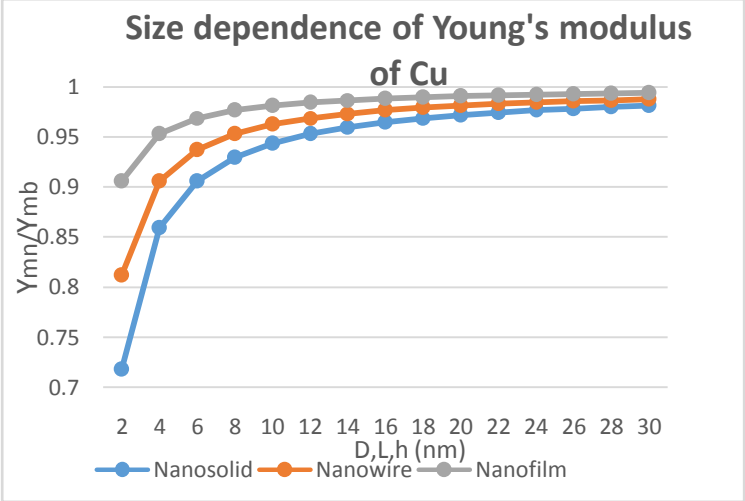


Fig. 1 Size dependence of Young's modulus of nanocrystalline Copper (Cu)

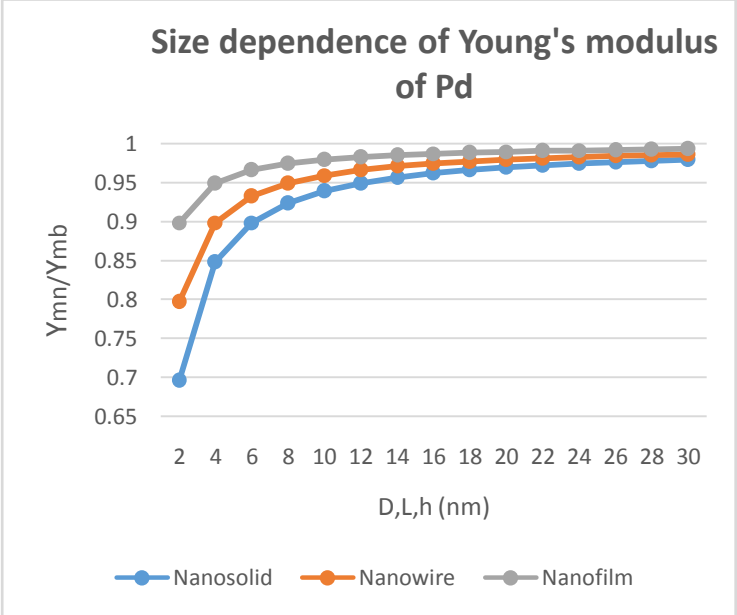


Fig. 2 Size dependence of Young's modulus of nanocrystalline Palladium (Pd)

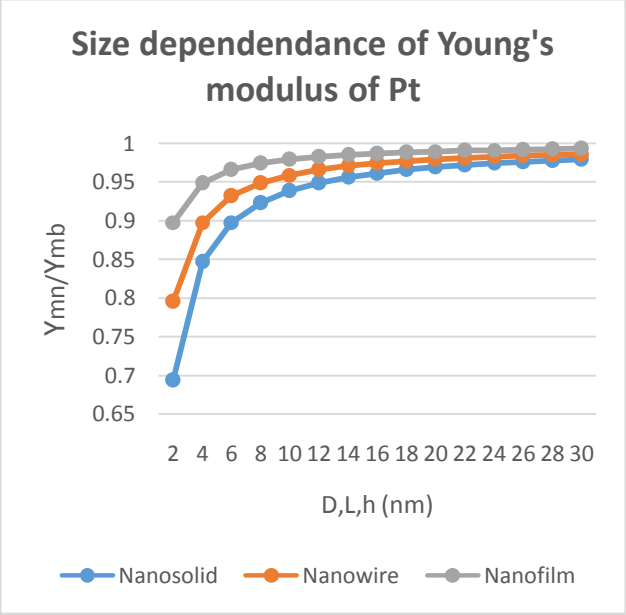


Fig. 3 Size dependence of Young's modulus of nanocrystalline Platinum (Pt)

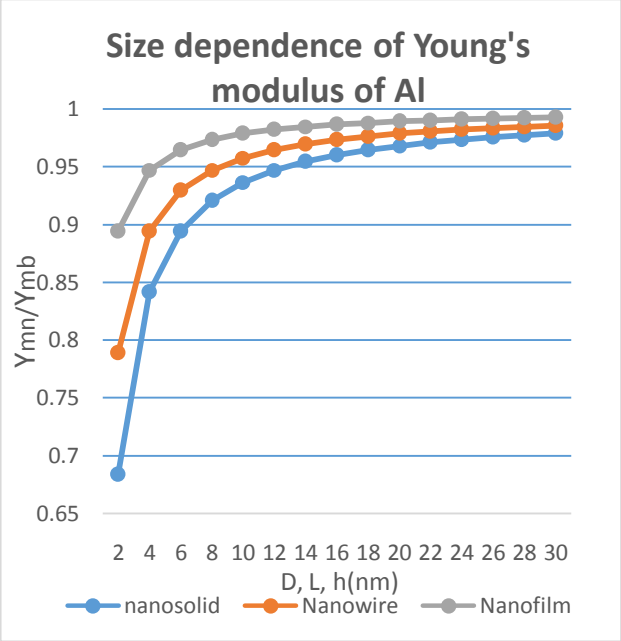


Fig. 4 Size dependence of Young's modulus of nanocrystalline Aluminium (Al)

**Conclusion:** In case of metallic nanostructured materials Young's modulus and Bulk modulus change gently with the variation of size and the curves are nearly horizontal for D >10 nm,which becomes very much prominent below 10 nm. Beyond 20 nm of the size of the material, the ratio of Young's modulus at nanoscale to the bulk becomes almost constant.

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