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Size and Shape Dependent Young Modulus and Vibrational Frequency of Nanomaterials

Vijay Veer[1], Raghuvesh Kumar[2]
Department of Physics, G.B. Pant University of Agriculture and Technology,
Pantnagar, Uttarakhand, India-263145

***Abstract-** A simple theoretical model is developed to study the size, shape and orientation dependence of Young modulus and vibrational frequency of nanomaterials. We have studied the Young modulus of Nano crystalline TiO_2, Si, Ag, Au and Cu for different shapes viz. spherical, nanowire and Nano film and the vibrational frequency of TiO_2 and Ag. The results obtained are compared with the available experimental data. A good agreement between theory and the experimental data supports the validity of the model developed.*

***Keywords-** Nanomaterial, Young modulus, Vibrational frequency, Size effect, Theoretical model*

I. INTRODUCTION

The elastic properties and the vibration characterization are important for the stability of materials and devices, especially for nanomaterials with potential and broad application. Nanomaterials show different properties from the corresponding bulk materials; the valid theoretical model about the size effect of the elastic modulus and the vibration frequency is significant to guide the application of nanomaterials [1]. Normally, the bulk value of Young modulus and vibrational frequency can be considered as a constant at a given temperature. However, in the nanoscale region, elastic modulus and vibrational frequency do not shows a universal variation trend as a function of D, where D denotes the diameter of a particle and a nanowire, or the thickness of a nanofilm. The variation trend depends strongly on the material and the application conditions such as temperature, atmosphere, and loading methods. Nanomaterials have large surface to volume ratio, and surface effect becomes important in the case of nanomaterials that is normally inconsequential for bulk materials. Liang *et al.* [2] used a molecular statics approach based on embedded atom method interatomic potentials to study the elasticityof copper nanowires along [001], [110] and [111] crystallographic directions. It has been found that for all three orientations, the surface is softer than an equivalently strained bulk and the overall nanowire softening or stiffening is determined by the orientation-dependent core elasticity. Yang and Zhao [3] studied size-dependent elasticproperties of a Ni nanofilm using molecular-dynamics simulations with the embedded-atom method. Lihong et al. [1] reported an analytical model for size-dependent elastic modulus and vibrational frequencies of nanocrystalline Cu, Ag, Si thin films and TiO_2 nanoparticles. Streitz et al. [4] studied the effect of size on the Young modulus of Ag nanofilm using computer simulation.Ao et al. [5] studied the effect of size on the Young modulus of Au and Cu nanowire at 0K and 300K and found that the trend of variation of elastic modulus with the size is different at the temperatures 0K and 300K. Cuenot et al. [6] studied the effect of reduced size on the elastic properties of silver and lead nanowires and polypyrole nanotubes with an outer diameter ranging between 30 nm and 250 nm. Resonant contact atomic force microscopy has been used to measure their apparent elastic modulus [6]. The measured modulus of the nanomaterials with smaller diameter is significantly higher than that of larger ones. This prediction has been explained on the basis of the surface tension effect. Lee and Rudd [7] as well as Omino et al. [8]reported the size dependence of the Young modulus for Si nanowires. Kumar and Kumar [9] developed a theoretical model to study the size dependent thermoelastic properties of metallic nanomaterials. Bhatt and Kumar [10] modified this model and found that the elastic modulus of nanomaterials depends on the size, shape and orientation of nanomaterials. Thus, elastic modulus is an important physical quantity in the case of nanomaterials which depends on the size, shape and orientation of nanomaterials.It seems that there is a lack of simple and straightforward method to study the size dependence of the elastic modulus and vibrational frequency.In the present paper; we develop a simpletheoretical model to study effect of size and shape the elastic modulus and vibrational frequency of nanomaterials which needs only one parameter. The formulation is given in the following section and the results and discussion in the next section.

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II. THEORETICAL FORMULATION

Bhatt and Kumar [10] developed the relation to study the size and shape dependence of Young modulus of nanomaterials, which reads as follows

$$\frac{Y\,(D)}{Y\,(\infty)}=\left(1\pm\frac{N_s}{2n}\right) \qquad (1)$$

where Y(D) is the Young modulus of nanomaterial with size D, $Y(\infty)$ elastic modulus of corresponding bulk material, N_s is the number of surface atoms and n is the total number of atoms.If N_i is the number of interior atoms,then n is N_s+N_i. Thus, we can write the eq. (1) as follows:

$$\frac{Y(D)}{Y(\infty)}=\left[1-\frac{1}{2\left(1\pm\frac{N_i}{N_s}\right)}\right] \qquad (2)$$

It has been discussed[11, 12] that the ratio of surface atoms to the interior atoms of a nanosolid can be expressed as $N_s/N_i=D_0/(D-D_0)$ [11, 12]. Here D_0 is a critical diameter for which all atoms of a nanosolid are located on its surface. Thus, we can write eq.(2) as follows

$$\frac{Y(D)}{Y(\infty)}=\left(1\pm\frac{D_0}{2D}\right) \qquad (3)$$

Here D_0 depends on dimensionality d and h through $D_0 = 2(3 - d)$has discussed earlier,[11, 12] where $d = 0$ for spherical nanosolid, $d = 1$ for nanowire, and $d= 2$ for nanofilm respectively. Here h is the atomic diameter, thus $D_0/2D$ is $3h/D$ for spherical nanosolids, $2h/D$ for nanowire and h/D for nanofilm. Thus, we can write the following relations for different type (shape) of nanomaterials using eq. (3).

Spherical nanosolid:

$$\frac{Y(D)}{Y(\infty)}=\left(1\pm\frac{3h}{D}\right) \qquad (4)$$

Nanowire:

$$\frac{Y(D)}{Y(\infty)}=\left(1\pm\frac{2h}{D}\right) \qquad (5)$$

Nanofilm:

$$\frac{Y(D)}{Y(\infty)}=\left(1\pm\frac{h}{D}\right) \qquad (6)$$

Now we discuss the effect of size and shape on the vibrational frequency of nanomaterials. Kumar and Kumar [13] developed a model to study the size and shape dependent vibrational frequency of nanomaterials. This model [13]is read as follows

$$\frac{\nu(D)}{\nu(\infty)}=\left(1-\frac{N_s}{2n}\right)^{1/2} \qquad (7)$$

where ν(D) is the vibrational frequency of nanomaterial with size D, $\nu(\infty)$ vibrational frequency of corresponding bulk material, N_s is the number of surface atoms and n is the total number of atoms.It is evidence that vibrational frequency does not show the universal trend of variation with size [1, 13]. Lihong *et al.* [1] show that the vibrational frequency decreases on increasing the size of the nanomaterial [1]. We may therefore write the expression for the vibrational frequency as follows:

$$\frac{\nu(D)}{\nu(\infty)} = \left(1 \pm \frac{N_s}{2n}\right)^{1/2} \tag{8}$$

Thus, we may write size dependent vibrational frequency of different shapes of nanomaterialsusing the value of $N_s/2n$ as discussed above:

Spherical nanosolid:

$$\frac{\nu(D)}{\nu(\infty)} = \left(1 \pm \frac{3h}{D}\right)^{1/2} \tag{9}$$

Nanowire:

$$\frac{\nu(D)}{\nu(\infty)} = \left(1 \pm \frac{2h}{D}\right)^{1/2} \tag{10}$$

Nanofilm:

$$\frac{\nu(D)}{\nu(\infty)} = \left(1 \pm \frac{h}{D}\right)^{1/2} \tag{11}$$

In the present paper we used these relations.

III. RESULT AND DISCUSSION

The input data [1,5] required for the present work are given in Table 1. We used eq. (4), eq. (5) and eq. (6) to compute the size dependent Young modulus of TiO_2, Si, Ag, Au and Cu for different shape viz. spherical, nanowire, and nanofilm. The results obtained are reported in figs. 1-5. Size dependence of the elastic modulus of TiO_2, Si and Ag using eq. (4), eq. (5) and eq. (6) is shown in the figs.1-3.The trend of variation of elastic modulus with size is similar for all the three shapes of these nanomaterials considered in the present paper. The experimental data [1] are available for TiO_2 (spherical), Si (nanofilm) and Ag (nanofilm) which have been included for comparison purposes. It should be mentioned that our model predictions agree well with the experimental data [1].It can be seen from Figs.1-3that the Young modulus decreases on increasing the size of the materials. We have computed the size dependence of the Young modulus of Au nanomaterial for different shapes viz. spherical, nanowire, and nanofilm using eq. (4), eq. (5) and eq. (6). The results obtained are reported in fig.4. The experimental data[5]are available for Au (nanowire) at 0Kwhich have been included for comparison purposes. It should be mentioned that our model predictions for Au nanowire are slightly higher than the experimental data [5] available at 0K. We also compared our results of Au nanowire with the theoretical results obtained by Ao *et al.* [5] at 300K. The trend of variation of our model is found similar to the theoretical results obtained by Ao et al. [5] at 300K. We have also computed the size dependence of the Young modulus of Cu nanomaterial for different shape viz. spherical, nanowire, and nanofilm using eq. (4), eq. (5) and eq. (6) The results obtained are compared with the experimental data[5]available at 0K for Cu (nanowire).Our model predictions for Cu nanowire are slightly higher than the experimental data [5] at 0K. We compared our results of Cu nanowire with the theoretical results obtained by Ao et al. [5] at 300K. The trend of variation of our model is found similar to the theoretical results obtained by Ao et al. [5] at 300K. It is found that $Y(D)/Y(\infty)$ tends to unity on increasing the size. This shows that the nanomaterial becomes bulk materials as size approaches about 100 nm. We studied the effect of size and shape on the vibrational frequency of TiO_2 and Ag nanomaterials using eq.(9), eq.(10) and eq.(11). The results obtained are reported in Figs. 6-7. The results obtained are compared with the available experimental data [1]. The experimental data [1] are available for TiO_2 nanoparticle and Ag nanofilm. The experimental data [1] are found slightly lower than the results obtained from eq.(9) and eq.(11).

IV. CONCLUSION

We have thus developed a simple theoretical model to study the size and shape dependence of Young modulus and vibrational frequency of nanomaterials. The model predictions are in good agreement with the available experimental data, which validate the proposed model. The beauty of our model is that it requires only one input parameter (h) which is easily available. Our model is applicable for metallic elements as well as compound nanomaterials. Our model explains the increasing and decreasing behavior of Young modulus and vibrational frequency with size. Due to the simplicity and applicability of the model, it may be extended to the other nanomaterials and may be of current interest to the researchers engaged in the study of other nanomaterials.

Table 1: Input parameters used in present work [1, 5]

S.No	Material	h(nm)
1	TiO_2	0.3239
2	Si	0.3368
3	Ag	0.2194
4	Au	0.2880
5	Cu	0.2760

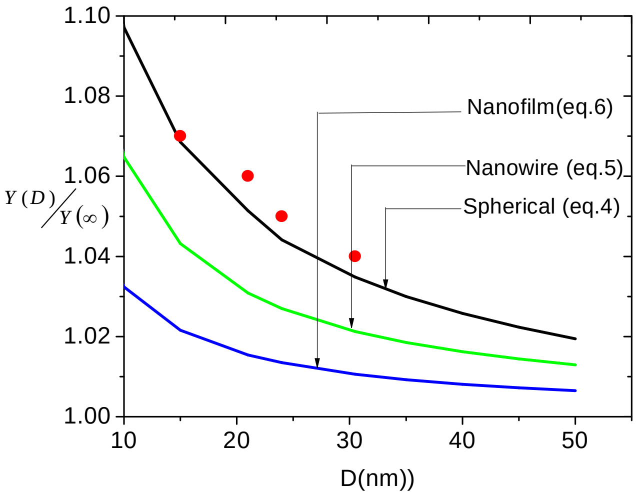


Fig. 1: Size and shape dependence of Young modulus of TiO_2 using eqs. (4-6).
The experimental data[1] are shown by ●for TiO_2 (spherical).

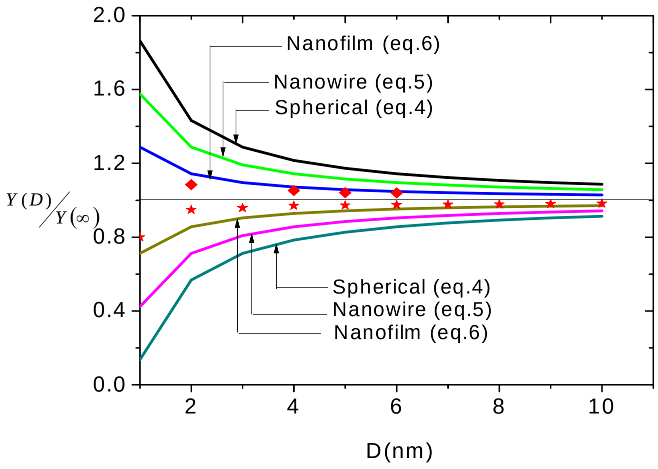


Fig. 2: Size and shape dependence of Young modulus of Si using eqs. (4-6).
The experimental data[1] are shown by ●for Si Nano film.

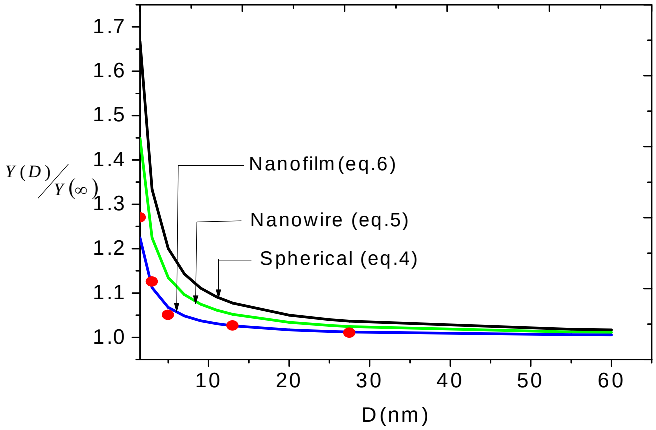


Fig. 3: Size and shape dependence of Young modulus of Ag using eqs. (4-6). The experimental data[1] are shown by ●for Ag nanofilm.

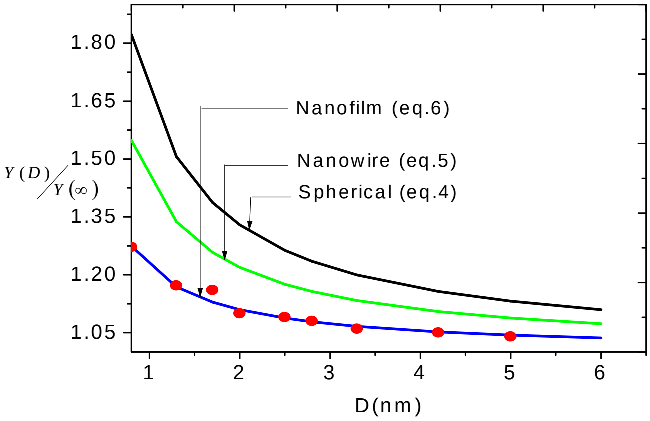


Fig. 4: Size and shape dependence of elastic modulus of Au using eqs. (4-6). The experimental data[5] are shown by ●for Au nanowire at 0K and ∗.are the theoretical results obtained by Ao *et al.* [5] at 300K.

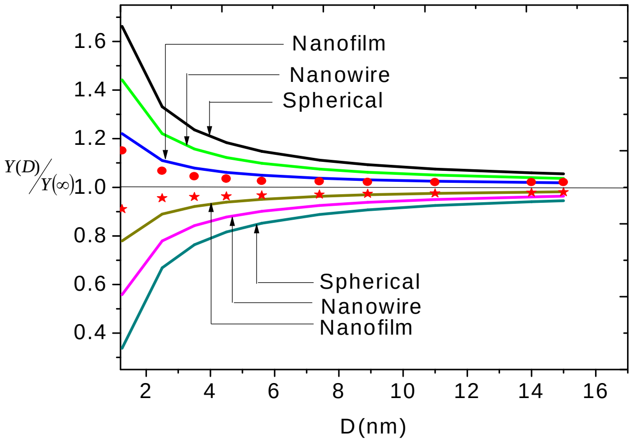


Fig.5: Size and shape dependence of Young modulus of Cu using eqs. (4-6). The experimental data [5] are shown by ●for Cu nanowire at 0K and ∗.are the theoretical results obtained by Ao*et al.* [5] at 300K.

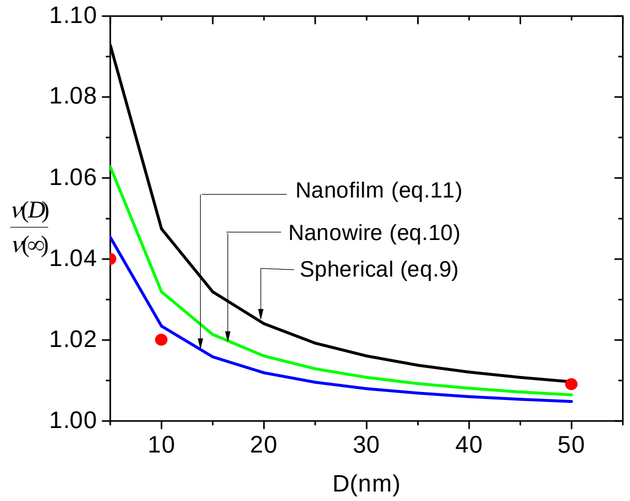


Fig. 6: Size and shape dependence of vibrational frequency of TiO_2 using eqs. (9-11).
The experimental data[1] are shown by ●for spherical.

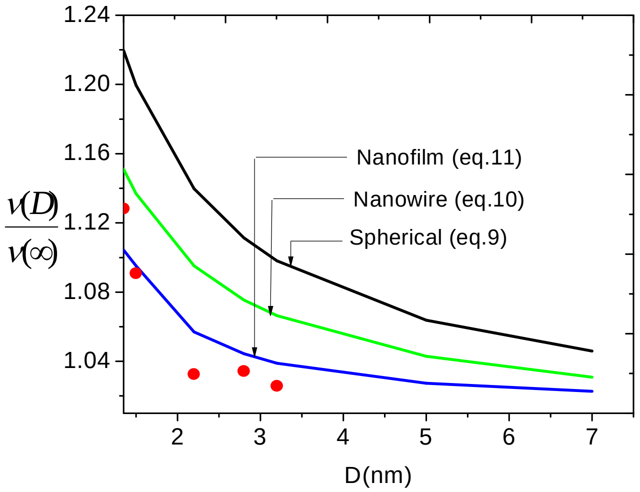
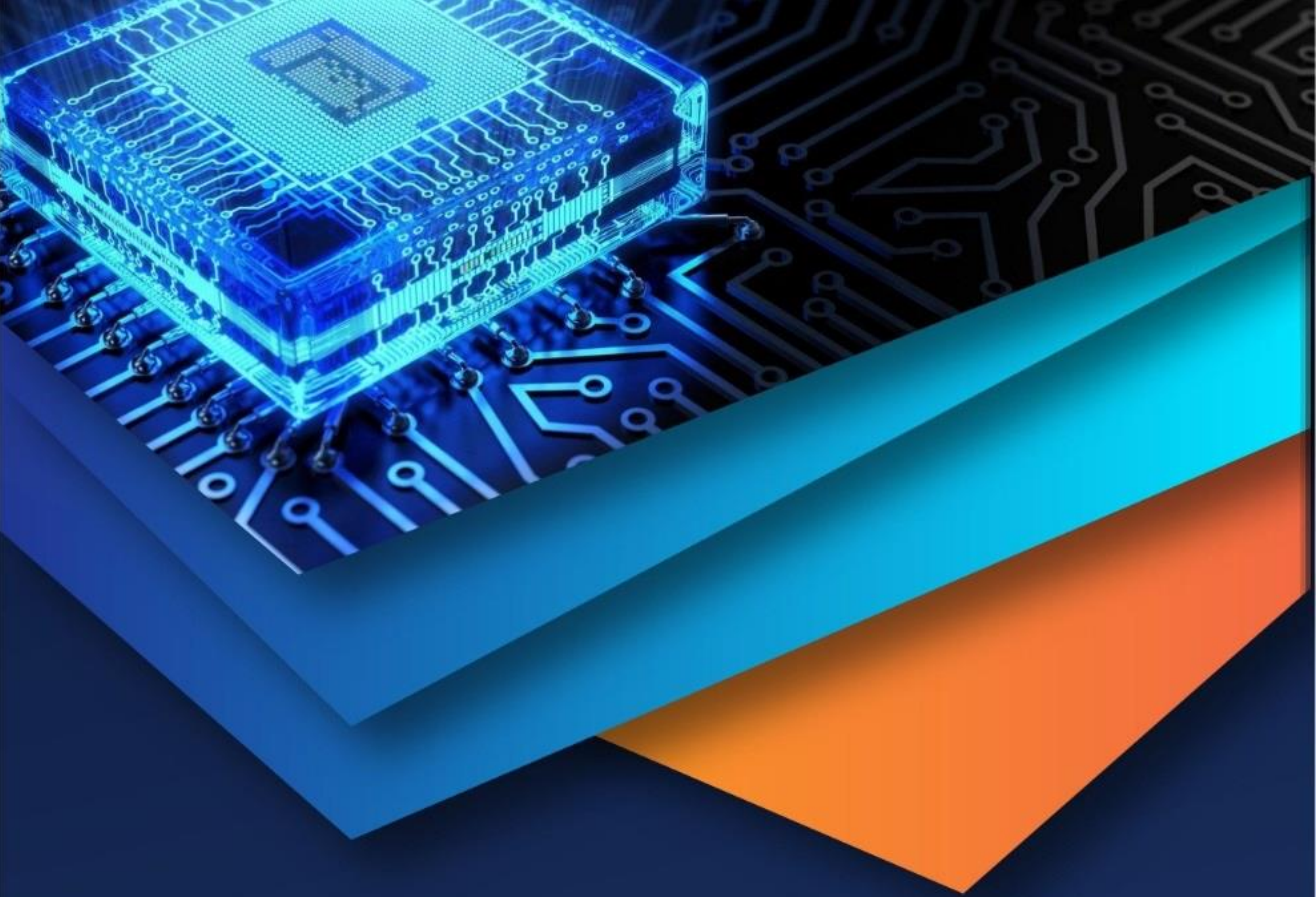


Fig. 7: Size and shape dependence of vibrational frequency of Ag using eqs. (9-11).
The experimental data[1] are shown by ●for nanofilm.

REFERENCES

[1] Liang, L. MA, H. and WEI, Y. Size-Dependent Elastic Modulus and Vibration Frequency of Nanocrystals , J. of Nanoscience., vol.2011, ID.670857, 2010.
[2] Liang, H. Upmanyu, M. and Huang, H. Size-dependent elasticity of nanowires: Nonlinear effects, Phys. Rev. B, vol.71, ID.241403, 2005.
[3] Yang, Z. and Zhao, Y. P. Size-dependent elastic properties of Ni nanofilms by molecular dynamics simulation, Surf. Rev. Lett.,vol.14, pp. 661, 2007.
[4] Streitz, F. H., Sieradzki, K. and Cammarata R. C. Size dependence young modulus of Ag nanofilm using computer simulation, Phys. Rev. B, vol.41, ID.2285, 1990.
[5] Ao, Z.M, Li, S. and Jiang, Q. The determination of Young's modulus in noble metal nanowires ,APL,vol. 93, ID. 081905, 2008.
[6] Cuenot, S.,Fretigny, C.,Champane, S. D. and Nysten, B. Surface tension effect on the mechanical properties of nanomaterials measured by atomic force microscopy, Phys. Rev. B, vol. 69, ID.165410, 2004.
[7] Lee, B. and Rudd, R. E. First-principles study of the Young's modulus of Si nanowires , Phys. Rev. B, vol.75,ID.041305, 2007.
[8] Omino,Y., Kuskima, A., Kitamurat., Gumbsch, P. and Li, L. Ab initio study of the surface properties and ideal strength of silicon thin films, Phys. Rev. B, vol.72 , ID.165431, 2005.
[9] Kumar, R., and Kumar, M. Size dependence of thermoelastic properties of nanomaterials, Int. J. Nano.,vol.9, pp. 537, 2010.

[10] Bhatt, A. and Kumar, M. Size and orientation dependence of elasticity of nanowire and nanofilm , EPL., vol. 99, ID.16001, 2012.
[11] Shif, G. Size dependent thermal vibration and melting in nanocrystals,J. Mater. Res.,vol.9,pp. 1307,1994.
[12] Jiang, Q., Shi, H. X., and Zha, M. Melting thermodynamics of organic nanocrystals, J.of Chem. Phy, vol.111, pp. 2176-2180, 1999.
[13] Kumar, R., Sharma, G., and Kumar, M. Effect of size and shape on the vibrational and thermodynamic properties of nanomaterials, J. Thermo., vol.1155, ID.328051, 2013.



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