Indian Journal of Pure & Applied Physics
Vol. 60, November 2022, pp. 951-955
DOI: 10.56042/ijpap.v60i11.63437

Application of Size and Shape Dependent Model for Shear Modulus of Nanomaterials

Varun Pandey* & Munish Kumar

Department of Physics, G.B. Pant University of Agriculture and Technology, Pantnagar 263 145, India

Received 20 May 2022; accepted 20 October 2022

A simple theory based on bond energy model is developed. The model is used to predict the size and shape dependence of shear modulus of different nanomaterials. The results obtained are compared with the our theoretical predictions as well as experimental data. In small size range (<10nm) there is a very good agreement between earlier predictions as well as experimental observations. It is discussed that present model is very simple as compared with the earlier model. In addition to this, our model includes the effect of shape also, which has not been considered in earlier theory. Due to the simplicity and applicability of the model, it can be used to understand the size and shape dependence of shear modulus of nanomaterials. To the best of our knowledge, such simple model is not yet available in the literature to predict the size and shape dependence of shear modulus.

Keywords: Shear modulus; nanomaterials; Size; Shape

1 Introduction

With a tremendous advancement in technology in the last few decades, the miniaturization of the matter has become possible and also the manipulation of the matter in such small scales. The field of nanoscience and nanotechnology has seen good growth and the effects of size reduction of matter has some unimaginable consequences as well. The reduction of the size of the matter to nanoscale has deep and unbelievable consequences. Almost all the properties show deviations in the trend that they follow at the macroscopic (bulk) scales[1-4]. As a result, a lot of work is in progress, both theoretically and experimentally to study the variations in the properties at nanoscale[5-15]. Elasticity is one of the most important properties in solids as it gives information about the hardness of the solid. The value of elastic constants does not remain constant with the reduction in size of the matter down to nanoscale[16-20]. There are some materials which are found to become harder as the size reduces and there are some which shows softness on the size reduction[21].

Claudio *et al.*[22] studied the effect of nano structurization on lattice dynamics of bulk nanocrystalline doped Silicon. The heat capacity, density of phonon states and elastic constants have been studied. Nanocrystalline-nanowires have been used in several applications[23]. To develop nanowire-based nano-devices, studies may be conducted on the characterization of the elastic properties and bulking strength of nanowire. The challenge associated with this seems due to the fact that the properties of nanowires are size dependent. To study the situation, Shaat & Abdelkefi[24] proposed a model to study the mechanics of nanocryastalline nanowire. The model has been used to study the bulking strength and the elastic properties of the nanowires made of nanocrystalline diamond, Si, Al, Cu, Ag, Au and Pt. However, it is well known that the properties of nanomaterials also dependent on shape, in addition to size[25,26]. Thus, it is legitimate and may be useful to propose a simple model, which includes the effect of shape in addition to size, which is the purpose of the present work.

2 Theory

Pandey & Kumar[27] reported the theory for the size and shape dependence of elastic behaviour of nanomaterials. The relation for bulk modulus has been reported as follows

$$\frac{B(n)}{B(b)} = \left(1 - \frac{\mathrm{N}}{2\mathrm{n}}\right)^4 \qquad \ldots(1)$$

where $B(n)$ is the bulk modulus of nanomaterial, $B(b)$ the bulk modulus of corresponding bulk material, N is the number of surface atoms and n the

*Corresponding authors:
(Email: email.to.varunpandey@gmail.com; munish_dixit@yahoo.com)

total number of atoms. It has been discussed that all the elastic moduli have similar trends of variation as shown by bulk modulus[28-30]. Thus, we can write,

$$\frac{S(n)}{S(b)} = \left(1 - \frac{\mathrm{N}}{2\mathrm{n}}\right)^4 \quad \ldots(2)$$

where S is the shear modulus, n and b represent nano and bulk respectively, $\frac{\mathrm{N}}{2\mathrm{n}}$ depends on size and shape of the nanomaterial, which may be computed using the method developed earlier[31]. These values have been compiled in Table. 1[31,32]. Thus, we can write the relations of shear modulus for different shapes of nanomaterials,

For Film: $\mathrm{S}(n) = \mathrm{S}(b)\left(1 - \frac{0.665d}{\mathrm{h}}\right)^4$ ...(3)

For Dodecahedral: $\mathrm{S}(n) = \mathrm{S}(b)\left(1 - \frac{0.898d}{a}\right)^4$ ...(4)

For Icosahedral: $\mathrm{S}(n) = \mathrm{S}(b)\left(1 - \frac{1.323d}{a}\right)^4$ ...(5)

For Wire: $\mathrm{S}(n) = \mathrm{S}(b)\left(1 - \frac{1.333d}{\mathrm{L}}\right)^4$ ...(6)

For Spherical: $\mathrm{S}(n) = \mathrm{S}(b)\left(1 - \frac{2d}{\mathrm{D}}\right)^4$ ...(7)

For Octahedral: $\mathrm{S}(n) = \mathrm{S}(b)\left(1 - \frac{2.449d}{a}\right)^4$ ...(8)

For Tetrahedral: $\mathrm{S}(n) = \mathrm{S}(b)\left(1 - \frac{4.898d}{a}\right)^4$ ...(9)

In these Equations, d is the atomic diameter, D,L,h,a the size of nanomaterials in respective shape. We used these relations in the present work to study the size and shape dependence of nanomaterials. The application of present model requires the shear modulus for bulk material, which is readily available in the literature. Thus, we can simply study the variation of shear modulus for different size and shape.

Table 1 — Input parameters used in present work[31,32].

Material	S(b) (GPa)	Atomic diameter d (nm)	Shape	N/n
Silicon	60	0.337	Film	1.33 *d/h*
Gold	26	0.332	Dodecahedral	1.796 *d/a*
Aluminium	24	0.286	Icosahedral	2.646 *d/a*
Iron	78	0.246	Wire	2.666 *d/L*
Diamond	440	0.183	Spherical	4 *d/D*
Platinum	62	0.350	Octahedral	4.898 *d/a*
Silver	24	0.344	Tetrahedral	9.797 *d/a*

Based on the bond energy model[33,34], cohesive energy of nanomaterial may be written as

$$E(n) = E(b)\left(1 - \delta\frac{\mathrm{N}}{\mathrm{n}}\right) \quad (10)$$

where $E(n)$ and $E(b)$ are the cohesive energies of nano and bulk material respectively. Following the concept that elastic moduli have the similar trends of variation[35] as that of cohesive energy, we can also write

$$S(n) = S(b)\left(1 - \delta\frac{\mathrm{N}}{\mathrm{n}}\right) \quad \ldots(11)$$

Here δ is the relaxation factor which may have the values ¼, ½ and ¾ as discussed by Qi[34]. Thus, we get

$$S(n) = S(b)\left(1 - \frac{\mathrm{N}}{4\mathrm{n}}\right) \quad \ldots(12)$$

$$S(n) = S(b)\left(1 - \frac{\mathrm{N}}{2\mathrm{n}}\right) \quad \ldots(13)$$

$$S(n) = S(b)\left(1 - \frac{3\mathrm{N}}{4\mathrm{n}}\right) \quad \ldots(14)$$

where N/n depends on the shape of nanomaterials as given in Table. 1. Thus, for example, Eqs. (12-14) for spherical shape may be written as

$$S(n) = S(b)\left(1 - \frac{\mathrm{d}}{D}\right) \quad \ldots(15)$$

$$S(n) = S(b)\left(1 - \frac{2\mathrm{d}}{D}\right) \quad \ldots(16)$$

$$S(n) = S(b)\left(1 - \frac{3\mathrm{d}}{D}\right) \quad \ldots(17)$$

Similarly, we can write the expressions of $S(n)$ for any shape of nanomaterial using Table. 1 which are used in the present work.

3 Results and discussion

The input parameters required for present work are compiled in Table. 1[31,32]. In the present paper, we have derived some simple relations to study the size and shape dependence of shear modulus for different types of nanomaterials. We selected those nanomaterials for which the experimental data are available so that model predictions can be judged. It is found that shear modulus decreases with the decreasing size. Different relations give similar trends of variation which justifies the applicability of each other. Moreover, the results based on Eq. (2) are

slightly smaller as compared with relations based on Eq. (10). This may be due to the different concepts involved in the two different approaches.

After Oxygen, Silicon is the most abundant element of Earth's crust. Due to its requirement, it has been widely studied. Claudio *et al.*[22] presented an experimental study of the elastic properties of Silicon. It has been observed that shear modulus is smaller than the single crystalline Si. Shatt & Abdelkefi[24] discussed that reporting the different properties of nanomaterials is a challenging task and a missing field of study. Having such idea in the mind, these authors reported the bulking strength and elastic properties of nanocrystalline materials. These results are included in Fig. 1. It is observed that Eq. (2) gives better agreement as compared with other relations. To confirm the situation, we have repeated our computational work for different nanocrystalline materials viz. Gold, Aluminum, Platinum, Silver. The results obtained are reported in Figs. 2-5 alongwith the results reported by Shatt & Abdelkefi[24]. In general, the trends of variation are similar with that reported earlier. In low size range (<10 nm), a good agreement is obtained with the earlier work[22,24]. It has been realized that the properties of nanomaterials are also shape dependent in addition to size [25,26]. In the present paper, we therefore extended the application of Eq. (2) for the study of shape effects. We developed Eq. (3-9) for this purpose. These equations

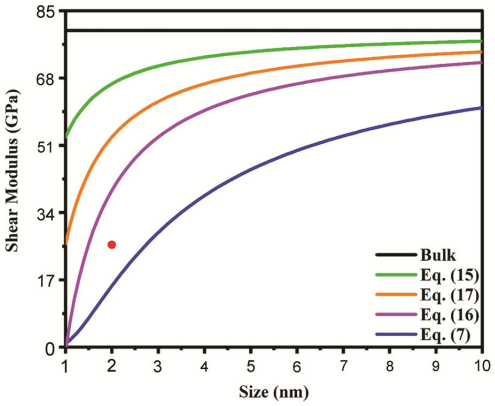

Fig. 1 — Size dependence of Shear modulus of spherical Silicon nanoparticles. ● [24].

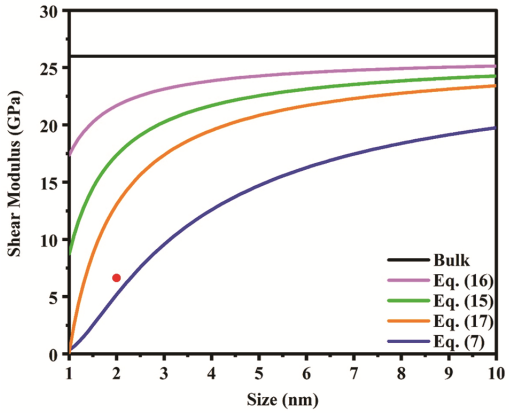

Fig. 2 — Size dependence of Shear modulus of spherical Gold nanoparticles. ● [24].

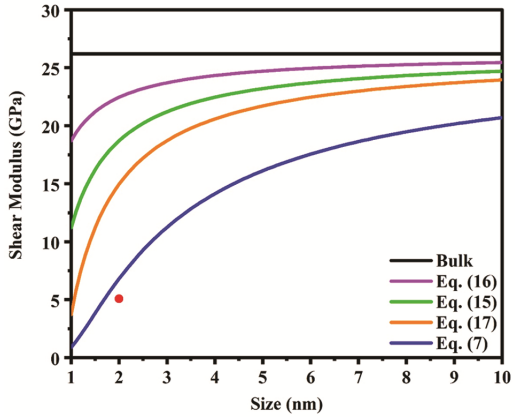

Fig. 3 — Size dependence of Shear modulus of spherical Aluminium nanoparticles. ● [24].

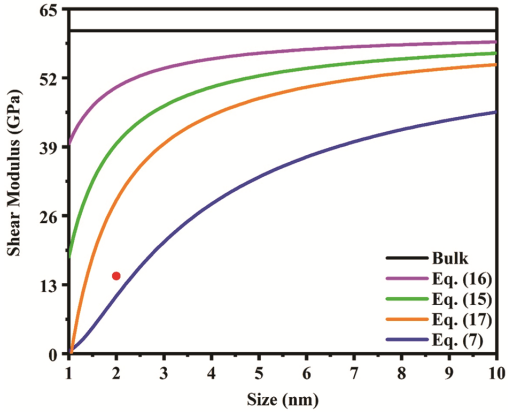

Fig. 4 — Size dependence of Shear modulus of spherical Platinum nanoparticles. ● [24].

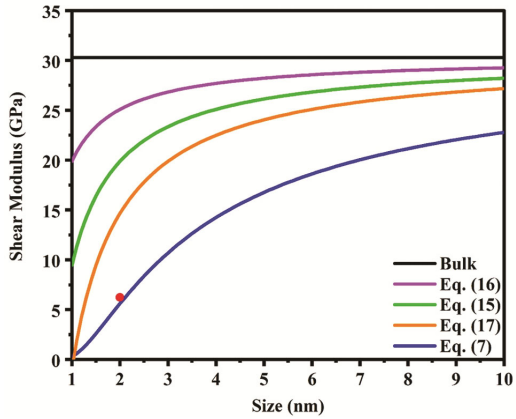

Fig. 5 — Size dependence of Shear modulus of spherical Silver nanoparticles. ● [24].

have been used for different shapes viz. Film, Dodecahedral, Icosahedral, Wire, Spherical, Octahedral and Tetrahedral. The results thus obtained are reported in Figs. 6-12 for different materials. A similar trend of variation is obtained. Shear modulus decreases with decreasing the size. For a particular size, the shear modulus has highest value for dodecahedral shape and minimum value for tetrahedral shape. For other shapes, the values are in between these two sets of data. This happens due to the increase of surface to volume atomic ratio by reducing the size. In the present model, this has been

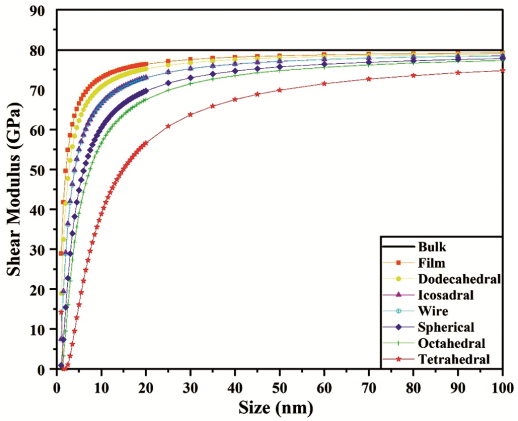

Fig. 6 — Size dependence of Shear modulus of Silicon for different shape using Eqs. (3-9).

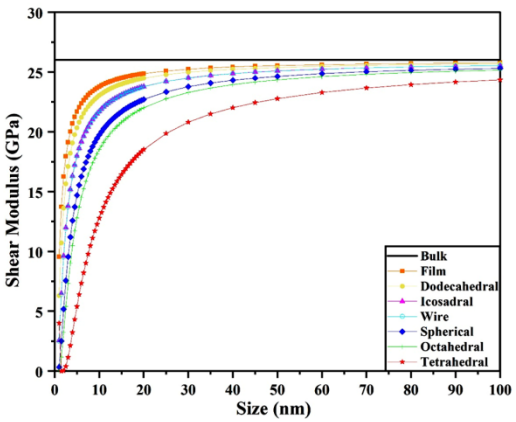

Fig. 7 — Size dependence of Shear modulus of Gold for different shape using Eqs. (3-9).

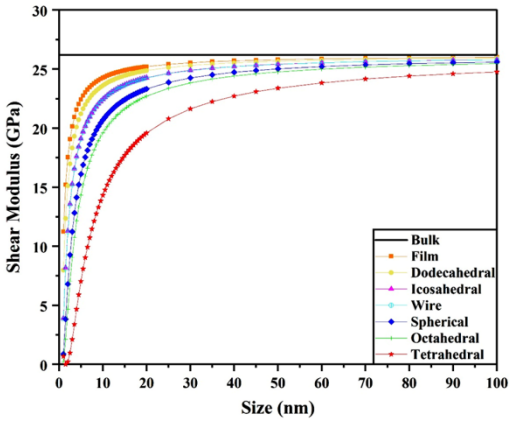

Fig. 8 — Size dependence of Shear modulus of Aluminium for different shape using Eqs. (3-9).

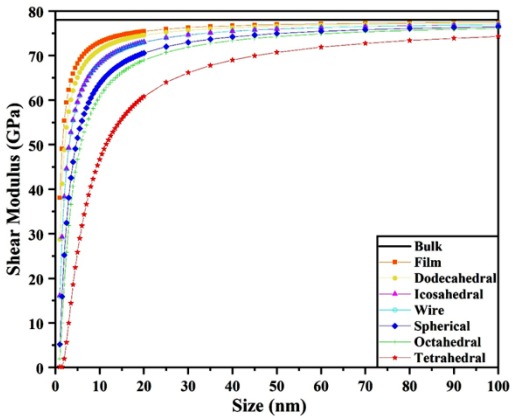

Fig. 9 — Size dependence of Shear modulus of Iron for different shape using Eqs. (3-9).

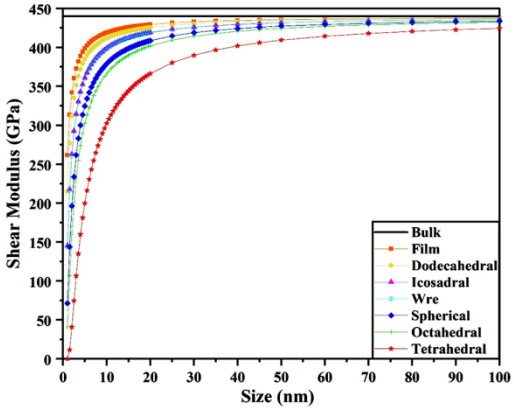

Fig. 10 — Size dependence of Shear modulus of Diamond for different shape using Eqs. (3-9).

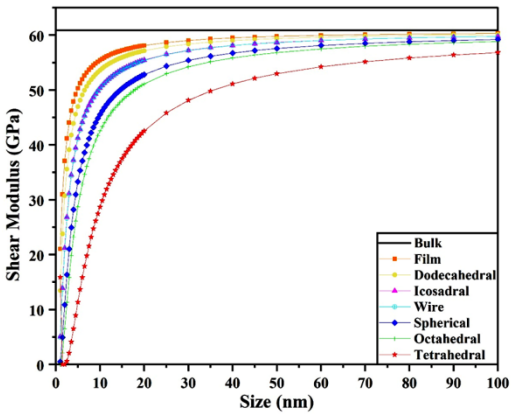

Fig. 11 — Size dependence of Shear modulus of Platinum for different shape using Eqs. (3-9).

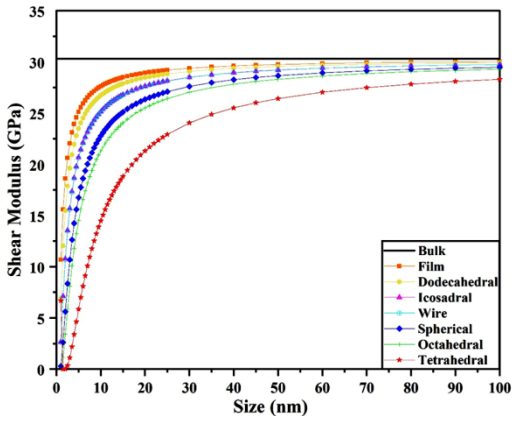

Fig. 12 — Size dependence of Shear modulus of Silver for different shape using Eqs. (3-9).

considered in the form of N/n. For all the shapes considered in the present work, shear modulus is less than the bulk value. It is observed that the effect of shape is much more prominent for low size and becomes less as size is increased with the material approaching the bulk behavior.

4 Conclusions

We have developed a simple model to study the size and shape dependence of shear modulus of nanomaterials. The results are discussed in the presence of earlier work. It is observed that shear modulus depends on size and shape. It decreases with decreasing size and have different values for different shapes. The results have been discussed in terms of surface to volume atomic ratio.

References

1 Guisbiers G & José-Yacaman M, Use of chemical functionalities to control stability of nanoparticles. In *Encyclopedia of Interfacial Chemistry: Surface Science and Electrochemistry,* Elsevier, (2018) 875.
2 Xiong S, *et al.*, *Phys Chem Chem Phys*, 13 (2011) 10652.
3 Guisbiers G, *Nanoscale Res Lett*, 5 (2010) 1132.
4 Yacamán M J, *et al.*, *Journal of Vacuum Science & Technology B: Microelectronics and Nanometer Structures Processing, Measurement, and Phenomena*, 19 (2001) 1091.
5 Qu Y D, *et al.*, *Phys Metals Metallogr*, 118 (2017) 528.
6 Zhu Y F, *et al.*, *J Phys Chem C*, 113 (2009) 16896.
7 Yang C C, *et al.*, *Solid State Commun*, 139 (2006) 148.
8 Zhao Y H & Lu K, *Phys Rev B*, 56 (1997) 14330.
9 Lee J G & Mori H, *The Europ Phys J D-Atom, Molecul, Opt Plasma Phys*, 34 (2005) 227.
10 Guisbiers G, Arscott S, Gaudet M, Belfiore A & Snyders R, Selenium surface energy determination from size-dependent considerations. In *IEEE 5th International Nanoelectronics Conference (INEC),* (2013) 105.
11 Qian L H, *et al.*, *Acta Mater*, 50 (2002) 3425.
12 Jiang Q, *et al.*, *Appl Phys A: Mater Sci Process*, 64 (1997).
13 Wang Z L, *et al.*, *J Phys Chem B*, 102 (1998) 6145.
14 Couchman P R & Jesser W A, *Nature*, 269 (1977) 481.
15 Hu J, *et al*, *Appl Phys Lett*, 86 (2005) 151915.
16 Liang L, *et al.*, *Philos Mag*, 93 (2013) 574.
17 Wang J, *et al.*, *J Phys D: Appl Phys*, 41 (2008) 165406.
18 Zhou X Y, *et al.*, *Phys Chem Chem Phys*, 18 (2016) 21508.
19 Yu X & Zhan Z. *Nanoscale Res Lett*, 9 (2014) 1.
20 Liu X J, *et al.*, *J Appl Phys*, 109 (2011) 074319.
21 Sharma G & Kumar M, *High Temp – High Press*, 44 (2015) 249.
22 Claudio T, *et al.*, *Phys Chem Chem Phys*, 16 (2014) 25701.
23 Cao G, *Nanostructures and nanomaterials: Synthesis and Applications*, Imperial Press, London, (2004).
24 Shaat M & Abdelkefi A, *J Appl Phys*, 120 (2016) 235104.
25 Lu H & Meng X, *Sci Rep*, 5 (2015) 1.
26 Chhabra H & Kumar M, *J Phys Chem Solids*, 139 (2020) 109308.
27 Pandey V, Kumar M, *Physica B: Condensed Matter*, 629 (2022) 413617.
28 Anderson O L, Equations of state of solids for geophysics and ceramic science (Oxford University Press, Oxford) 1995.
29 Kumar M, *Physica B*, 311 (2002) 340.
30 Bhatt S & Kumar M, *High Temp- High Press*, 47 (2018) 383.
31 Bhatt S & Kumar M, *J Phys Chem Solids*, 106 (2017) 112.
32 Qi W H & Wang M P, *J Nano Res*, 7 (2005) 51.
33 Qi W H, *Physica B: Condensed Matter*, 368 (2005) 46.
34 Qi W, *Nanoscop Thermodyn, Accounts Chem Res*, 49 (2016) 1587.
35 Kumar R & Kumar M, *Int J Nanosci*, 9 (2010) 537.