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LETTER TO THE EDITOR

Analysis of the paper: "Modeling to determine bulk modulus dependence on size, shape and dimensionality of nanomaterials" by M. Goyal [High Temperatures – High Pressures 52, 465(2023)]

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The model presented by Goyal [High Temperatures – High Pressures 52, 465 (2023)] to study shape, size and dimension effect on the bulk modulus of nanomaterials has been copied from Physica B 629, 413617 (2022) and the expression of size dependence of melting temperature from [J. Phys. Chem. C 113, 7598 (2009)]. The frequently used words by the author "a simple model presented" or "In view of model proposed" are misleading to the readers and infringe on the rights of others.

Recently, Pandey and Kumar [1] first time reported the theory of nanomaterials, which relates the bulk modulus of nanomaterials with their melting temperature as given below:

$$\frac{B_n}{B_b} = \left(\frac{T_{mn}}{T_{mb}}\right)^2 \tag{1}$$

where B_n and B_b are the bulk modulus of nano and bulk material respectively and T_{mn} and T_{mb} are corresponding melting temperature. Goyal [2] copied entire formulation of Eq. (1) from Pandey and Kumar [1] and wrote very clearly in abstract "a simple model is presented", "In view of model

proposed". Thus, it seems that Eq. (1) emerge out from the study of Goyal [2], which is misleading to readers.

Pandey and Kumar wrote, "It is very clear that the size and shape dependence of bulk modulus of nanomaterials may be studied by the knowledge of size and shape dependence of the melting temperature".

Inspired from this Goyal [2] further copied the Eq. (5) of Lu et al [3], which reads as follows

$$\frac{T_{mn}}{T_{mb}} = \left\{1 - \frac{1}{\left(\frac{12D}{D_0} - 1\right)}\right\} exp\left\{-\frac{2\alpha S_b}{3R\left(\frac{12D}{D_0} - 1\right)}\right\} \tag{2}$$

Combination of Eq. (1) and Eq. (2) gives

$$\frac{B_n}{B_b} = \left[\left\{1 - \frac{1}{\left(\frac{12D}{D_0} - 1\right)}\right\} exp\left\{-\frac{2\alpha S_b}{3R\left(\frac{12D}{D_0} - 1\right)}\right\}\right]^2 \tag{3}$$

This replaces the following relation of size dependence of melting temperature used by Pandey and Kumar [1] based on the bond energy model as proposed by Bhatt and Kumar, which reads as [4]

$$\frac{T_{mn}}{T_{mb}} = \left(1 - \frac{N}{2n}\right)^k \tag{4}$$

which gives (using Eq. 1)

$$\frac{B_n}{B_b} = \left(1 - \frac{N}{2n}\right)^{2k} \tag{5}$$

where the terms have their usual meaning as defined earlier [1]. In the present analysis we used the same notations as used by Goyal [2] to avoid any confusion. The model depends on the size dependence of melting temperature. Therefore, we must discuss the models of melting temperatures before proceeding to the other properties [2].

Now, it is pertinent to mention here that a number of relations for the size dependence of melting temperature are available in the literature [3–6]. Thus, by changing the relation of melting temperature in the theory as proposed by Pandey and Kumar [1] gives several relations in place of Eq. (5). What does it mean. Is there any improvement in theory. Here we address this point.

Actually, before proceeding with Eq. (4) for elastic properties [1], the other relations for melting temperature were discussed in detail [4–6]. Not only this, more recently we provided a comparative study of these equations during the study of size and shape dependence of band gap [7]. It has been observed that the theory based on Eq. (4) gives the better agreement with the available experimental data as compared with that based on Eq. (2). Moreover, for present analysis, we used Eq. (2) and Eq. (4) to demonstrate the size dependence of melting temperature of nanomaterials using the input parameters as given by Lu et al [8]. The results obtained are reported in Figs. 1–5 with available experimental data [9–13] which is crucial in the study of Goyal [2]. This clearly demonstrates that Eq. (4) gives better results as compared with Eq. (2). Thus, to replace Eq. (4) by Eq. (2) for properties of nanomaterials which depend on melting temperature is not justified as presented by Goyal [2].

TABLE 1
Input parameters used in the present work [8]

S. No.	Material	Atomic Diameter d (nm)	Melting temperature T_{mb} (K)	S_b (J/K-mol)
1.	Ag	0.289	1235	7.82
2.	Al	0.286	933	6.15
3.	Au	0.288	1337	7.62
4.	Pb	0.350	601	6.65
5.	Sn	0.324	505	9.22

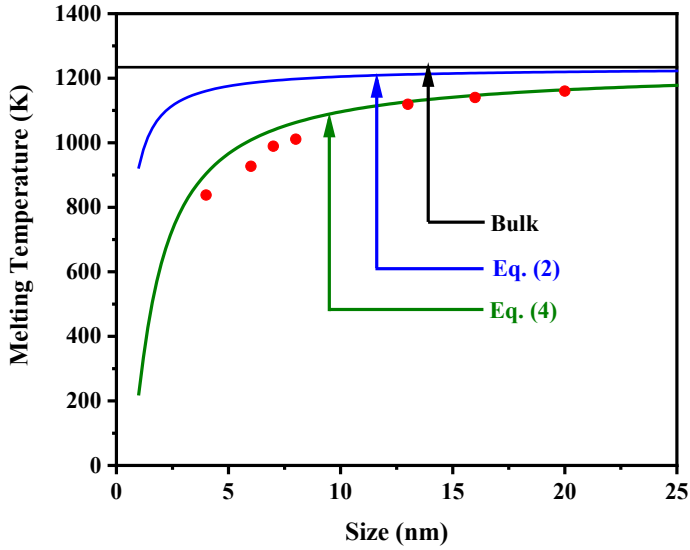

FIGURE 1
Size dependence of melting temperature of Ag nanoparticle • represent experimental data [9].

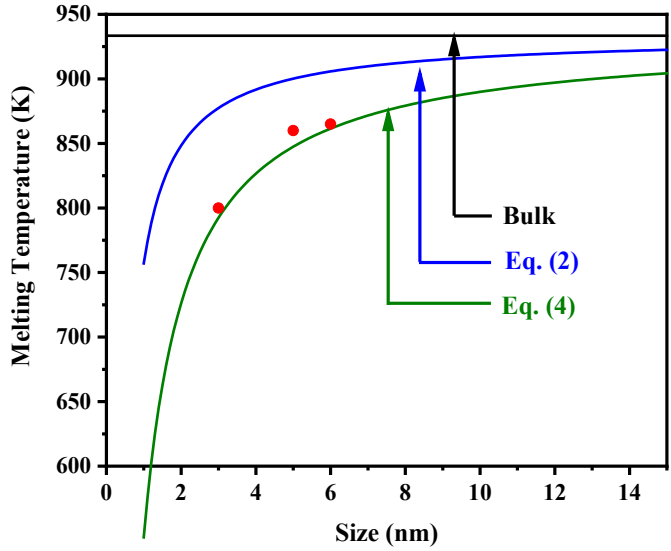

FIGURE 2
Size dependence of melting temperature of Al nanoparticle • represent experimental data [10].

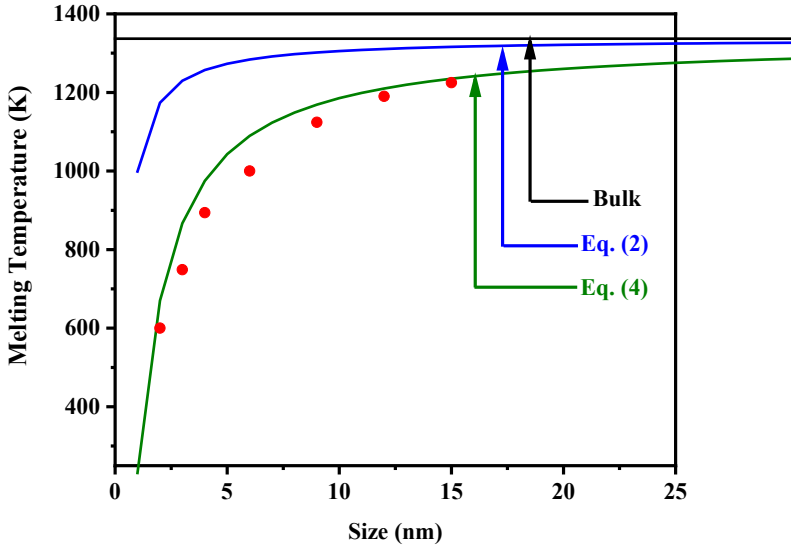

FIGURE 3
Size dependence of melting temperature of Au nanoparticle • represent experimental data [11].

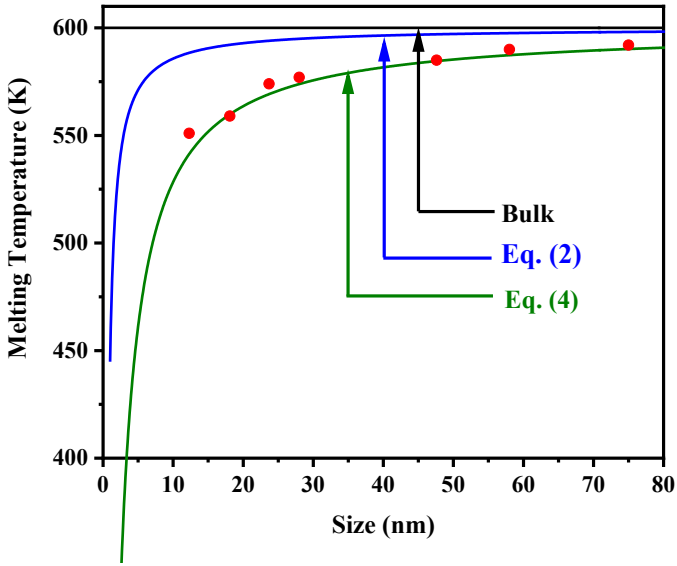

FIGURE 4
Size dependence of melting temperature of Pb nanoparticle • represent experimental data [12].

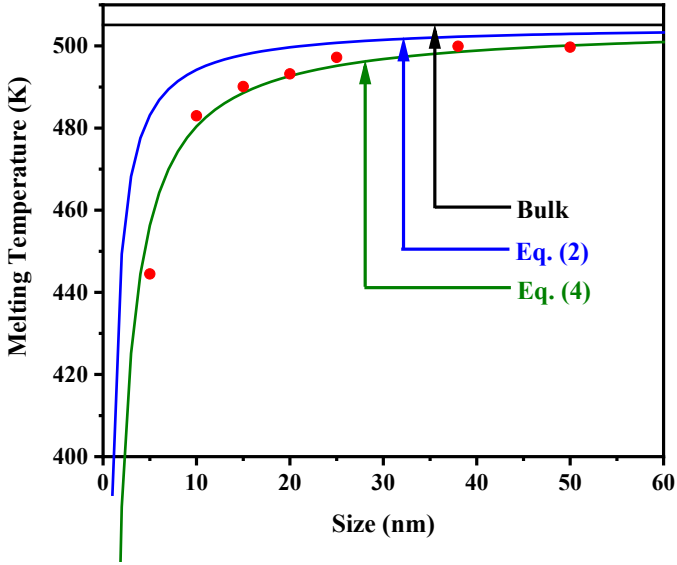

FIGURE 5
Size dependence of melting temperature of Sn nanoparticle • represent experimental data [13].

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AUTHOR'S RESPONSE

It is highly objectionable to use the words like copied and misleading in this LETTER. The relations used by Goyal [High Temperatures- High Pressures 52, 465(2023)] in article are both cited in the published paper as ref. [23, 24]. It is not appropriate to say that model is copied from the citation given. Bulk modulus expression presented in Goyal [High Temperature- High Pressure 52, 465(2023)] for nanocrystals obtained using Lu et al. [24, 25] expression for melting temperature of nanocrystals is not used by any of the previous workers to my knowledge. Therefore, I think there should be no problem with the working model proposed. Also, melting temperature expression proposed by Lu et al. [24, 25] is cited in my article. Bulk modulus relation with group velocity and mass density is used in Goyal manuscript and wherever required proper citations are all given. Citations given are not only of Pandey and Kumar [23] but also of Abdullah et al. [22]. It is clearly mentioned in my paper that "The relation of bulk modulus dependence on group velocity and mass density in solid materials is extended for nanomaterials and using melting temperature expression, the relation of bulk modulus of nanomaterials is obtained in terms of size, shape factor and dimension. The melting temperature expression proposed by Lu et al. [24] is used to find bulk modulus relation for nanomaterials".

It is asked in this letter whether my work is improvement in theory. In my paper, I have not done the comparison of the model results with the previous models so it cannot be said that which model results are better. There are different qualitative and quantitative approaches available in the literature. If the theoretical study of particular thermophysical parameter is done using a specific approach, it does not mean that other approaches can not be used for studying the same thermophysical property. Comparative study can be done in further studies if required.

In this letter, authors depict the melting temperature variation in Ag, Al, Au, Pb and Sn nanoparticles with respect to size using the Lu et al. [24] expression and Bhatt & Kumar proposed expression. However In my paper, the bulk modulus variation in nanomaterials of different dimensions with respect to size is studied for nanomaterials of Si, Cu, Al, Au, Ag, Pt.

The remark *"Thus, to replace Eq. (4) by Eq. (2) for properties of nanomaterials which depend on melting temperature is not justified as presented by Goyal [2]" is also objectionable*. In my study, I do not conclude that melting temperature expression proposed by Bhatt and Kumar is to be replaced by Lu et al. [24] expression of melting temperature of nanocrystals. The parameter computed in my study is different from that of Bhatt and Kumar study.

Overall, it is highly objectionable to use words like copied, misleading, and not justified in this letter to the Editor.

M. Goyal