Effect of Size and Shape on Young's Modulus of Nanostructured Ag by Lindemann's Criterion

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Abstract

A simple theoretical model based on the Lindemann's criterion has been explored to account for size and shape dependent Young's modulus of silver (Ag) nanostructures (NSs). The shapes of Ag NSs considered herein are nanoparticles (NPs), nanowires (NWs) and nanofilms (NFs). It is found that Young's modulus of these Ag NSs show a nonlinear variation with respect to the smallest dimension of the structure and depressed gradually. The model predictions for the Young's modulus of Ag NSs are consistent with reported experimental results. This supports the validity of the model explored.

Keywords: Silver, Nanostructure, Size, shape, Young's modulus

Introduction

It is well accepted that size matters when specimen is small enough. Properties of nanostructures (NSs) vary with size. NSs have different properties from the bulk due to their high surface area over volume ratio and possible appearance of quantum effects at the nanoscale [1]. Various physical properties such as cohesive energy, melting temperature, Debye temperature etc. are strongly dependent upon particle size [2]. Zhao et al.[3] studied the size dependence of bulk modulus of nanocrystalline Ni by means of molecular dynamics simulation. Yang and Zhao [4] studied the size-dependent elastic properties of Ni nanofilms using molecular dynamics simulation. Lee and Rudd [5] as well as Omino et al. [6] reported the size dependence of the Young's modulus for Si nanowires. Theoretical method to study the size dependence of bulk modulus has been explored by Kumar and Kumar [7]. Bhatt and Kumar [8] studied the size dependent bulk modulus and equation of state for different NSs. Recently, there are also evidences that elasticity of NSs depends on the size [9].

Within the framework of elasticity, Young's modulus is one of the most significant parameter. It determines the basic elastic deformation capacity of a material under a bear load. The bulk value of the Young's modulus may be considered as a constant for a particular pressure and temperature. Moreover; for NSs, Young's modulus does not show a universal trend with particle size. The variation trends depend strongly on the application conditions. Thus, it seems that there is a lack of simple and straightforward method to study the size dependence of the Young's modulus. A unified model for size-dependent materials properties is developed based on the Lindemann criterion [10]. The model has predicted the

size-dependent properties of nanoparticles (NPs), nanowiews (NWs) and nanofilms (NFs). The purpose of present paper is thus to study size-dependence of Young's modulus for Ag-NSs.

Theory

Based on Lindemann's criterion of melting, the size dependent melting temperature can be determined. The detailed analysis is given elsewhere but mathematical form reads as follows:

$$T_n(r)/T_b(\infty) = exp[\pm(\alpha - 1)/(r/r_0 - 1)] \quad \ldots (1)$$

where $T_n(r)$ and $T_b(\infty)$ are the melting temperature of the NSs with smallest dimension r and corresponding bulk value respectively. r_0 denotes a critical radius at which all atoms of the NSs located on its surface. Positive and negative signs may be taken according to the orientations. α is defined as the ratio of the mean square displacement (msd) of atoms on the surface and that in the interior of NSs. For low dimensional NSs, r_0 is dependent on the its dimension d: $d = 0$ for NPs, $d = 1$ for NWs and $d = 2$ for NFs. In general, the dimension can be fractional. For a NP, d has the usual meaning of its radius. For a NW, d is taken as its radius and for a NF, d denotes its half thickness. d_0 is given by: (1) $r_0 = 3h$, for $d = 0$ since $4\pi r_0^2 h = 4\pi r_0^3/3$; (2) $r_0 = 2h$, for $d = 1$ since $2\pi r_0 h = \pi r_0^2$; (3) $r_0 = h$, for $d = h$ since $2h = 2r_0$. In short, the relationship between d and r_0 is

$$r_0 = (3 - d)h \quad \ldots (2)$$

Note that if the crystalline structure or co-ordination number of a crystal is different, h varies somewhat. It is evident from Eq. (1) that $T_m(r)$ function depends on α. If $\alpha > 1$, $T_n(r)/T_b(\infty) < 1$, $T_n(r)$ increases as r increases and opposite istrue, if $\alpha < 1$. For crystals with free surfaces, such as free-standing particles, nanowires in porous glasses and thin films deposited on inert substrates, msd of the surface atoms is larger than that of the interior atoms of the nanocrystals and $\alpha > 1$. α can be deduced by the by the vibrational entropy expression is expressed as [11]

$$\alpha = [2S_{vib}/3R] + 1 \quad \ldots (3)$$

where R is the ideal gas constant. For metallic NSs, $S_{vib} \approx S_m(\infty)$, with $S_m(\infty)$ as bulk melting entropy.

Following Qi's model explored [9], we may write the expression for Young's modulus of NSs as

$$Y_n(r)/Y_b(\infty) = exp[\pm(\alpha - 1)/(r/r_0 - 1)] \quad \ldots (4)$$

where $Y_n(r)$ and $Y_b(\infty)$ are the Young's modulus of the NSs with smallest dimension r and corresponding bulk value respectively. In the present paper, we used Eq. (4) to compute the Young's modulus of Ag-NPs, Ag-NWs and Ag-NFs, respectively.

Results and Discussion

Bhatt and Kumar [8,9] studied the size dependence of Young's modulus of different nanostructures using Qi's model [12]. This encouraged the authors to explore the model based on Lindemann's criterion for Young's modulus of Ag-NSs.

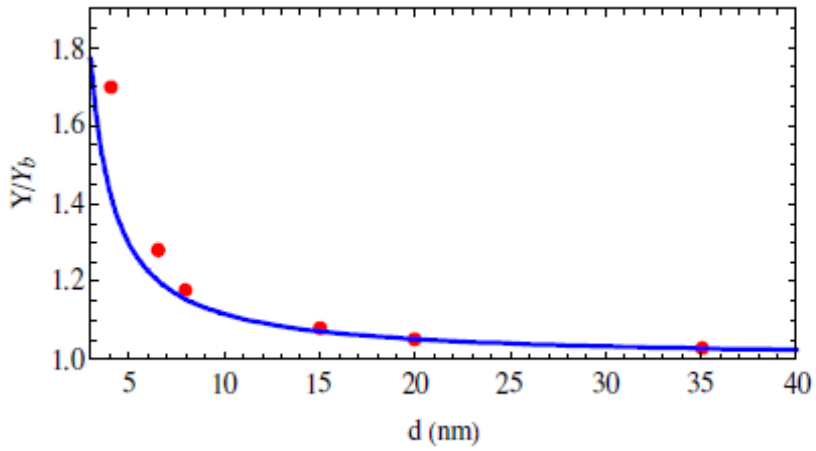

Fig. 1 Size dependence of Young's modulus of Ag-NPs. Symbol denotes the experimental values [13,14].

Fig. 1 presents the size dependent Young's modulus of Ag-NPs. As obvious, the Young's modulus increases as we go down the particle size. It is clear from Fig. 1 that the size effect on Young's modulus is more and more obvious with the decrease in size. The relevant curve can be divided into two parts, sizes greater than $10\ nm$ and sizes less than $10\ nm$. Young's modulus changes gently with the variation of size and the curves are nearly horizontal for $D > 10\ nm$. However, on the contrary, the size effect is very distinct in the range of $D < 10\ nm$. Young's modulus increases sharply with further small reduction of particle size. Our results are in good agreement with experimental data [13,14].

The size dependence of Young's modulus of Ag-NWs is shown in Fig. 2. It is seen that the Young's modulus of Ag-NWs decreases on increasing the diameter of wire. We compared our results with the available experimental data [15]. It is observed that the trend of variation is noteworthy below $100\ nm$. Moreover, our results agree well with experimental data [15].

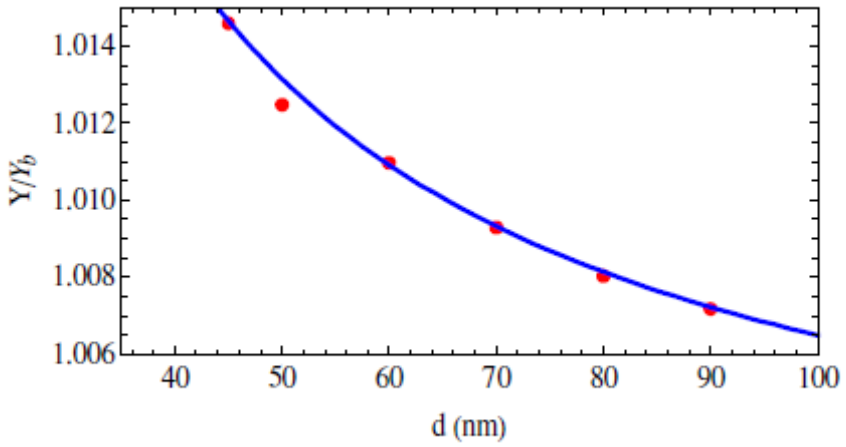

Fig. 2 Size dependence of Young's modulus of Ag-NWs. Symbol denotes the experimental values [15].

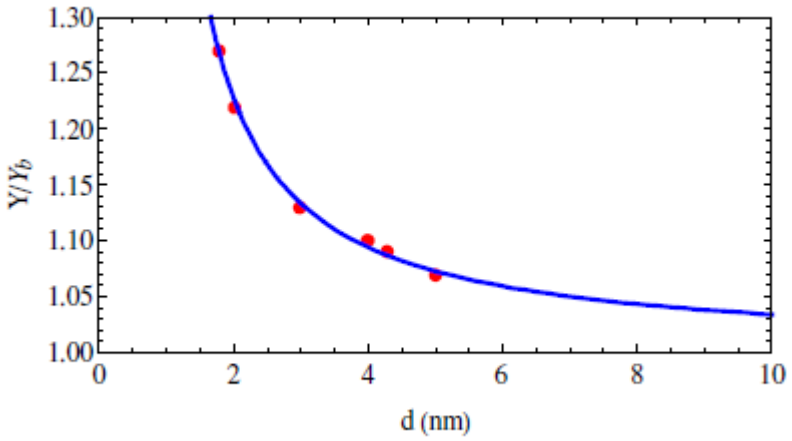

Fig. 3 Size dependence of Young's modulus of Ag-NFs. Symbol denotes the computer simulation [16].

The computed values of Young's modulus for Ag-NFs are displayed in Fig. 3 along with the `computer simulation` [16]. There is good agreement in the present work with simulation results [16]. This demonstrates the suitability of the model explored. It is found from above stated figures that Y_n/Y_b is very close to unity. Nanomaterial becomes bulk material as smallest dimension of NSs approaches below some particular value. It is also obvious that trend of variation of Young's modulus with shape of NSs is noteworthy. This is due to the known fact that the different dimensions of NSs have different surface/volume ratios.

Conclusion

In conclusion, a simple model using Lindemann's criterion is used to account for the size dependence of the Young's modulus of Ag-NSs. Calculated values of Young's modulus of Ag-NSs using Lindemann's criterion are found in reasonable agreement with available experimental and simulation results that suggests the validity of our results. It is finally developed that Lindemann's theory can successfully be used to study the other size dependent elastic properties of nanostructures.

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