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EFFECT OF SIZE ON DEBYE TEMPERATURE OF AU AND CU NANOMATERIALS

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ABSTRACT

By studying the surface effect, the Debye temperature of nano solids (nano particles, nano wires, nano films) has been predicted based on surface dependent cohesive energy. Nano size material shows many motivating properties that cannot be seen from their bulk equivalent. The cause for the size dependent properties of the nano materials is observed as the presence of the large fraction of the surface atoms. Because, free surface atoms experience a different environment than do atoms in the bulk of the materials. As a consequence, the energy associated with these atoms is different from that of atoms in the bulk. In this paper, on exposing the surface effect, the Debye temperature of the Au and Cu nano materials of nano sphere, nano wire and nano film has been studied based on particle size dependent cohesive energy. It is observed that Debye temperature decreases with the decrease in grain size. Furthermore, the Debye temperature increases for nano wire and nano film as compared with the spherical form of same size

Keywords: Nano Materials, Debye Temperature, Cohesive Energy

I. INTRODUCTION

When the particle size of materials transforms the nanometre scale, the electronic, magnetic, biomedical and thermodynamic properties vary noticeably as compared with its bulk counterparts [1, 2]. The important characteristics of the nano materials are its size effects. It is recognized that the size dependence of thermal stability in nano materials is increasingly becoming one of the major concerns in upcoming technologies [3]. Numerous experimental and theoretical efforts have been implemented to investigate the size-dependent cohesive energy of nano materials [4]. Size dependence of cohesive energy of W was carried out by Kim *et al*. [5]. Cohesive energy of Ag and Co nano particles is studied by Hou *et al*. [6] using computer simulations. Gold and silver at the nano scale have demonstrated many intriguing chemical and physical properties that their bulk counterparts do not have. The size dependent elastic modulus of Cu and Au thin film studied by Liang *et al*. [7] and suggested that the elastic modulus of metallic free thin films increases as the thickness of the film increases. Size dependent melting behavior of Zn nano wire using X ray diffraction and transmission electron microscopy studied by Wang *et al*. [8]. The size dependence melting temperature of Au nano material has been studied and it is shown that the melting temperature decreases as the size decreases [9]. Nano materials are inspiring since they reveal strong size and shape effect which cannot be defended by the traditional theories. Extensive theoretical and vibration of atoms.

In the present work, we report a theoretical model for studying the grain size dependent Debye temperature of Au and experimental investigations have been executed by the researchers in reviewing the special properties of nano materials [7-9] and motivating results have been obtained.

Counting these properties of nano materials, the Debye temperature of nano materials has received great attention, because it is a central physical quantity to characterize many material properties, such as phase transitions and thermal Cunano solids in different shapes such as nano particles, nano wires, and nano films with free surface. The study based on surface effect at decreased grain size, licences interpolation and extrapolation to the region for which adequate experimental data are not available. The model predictions agree well with the available experimental data.

1.2 Theoretical Formulation

The entire cohesive energy of the nano materials is due to the involvement of the surface atoms as well as the interior atoms may be listed as [10]

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

Where n is the total number of atoms of nanosolids and the number of its surface atoms is N .Consequently, $(n - N)$ is the total number of interiors atoms of the nanomaterials. E_0 is the cohesive energy of the bulk materials per atom. Eq. (1) may be inscribedequally

$$E_p = E_b(1 - \frac{N}{2n}),$$

Where E_p is the cohesive energy per mole of the nanomaterials, which is given by AE_{total} / n , here, A is the Avogadro constant. E_b is defined as the cohesive energy per mole of the corresponding bulk materials which is given by $E_b = AE_0$ .The relation between the melting point of nanomaterials and bulk are reported by Qi [10] as: $T_p = T_b\left(1 - \frac{N}{2n}\right)$ (2)

One may get the connection between the melting point and the Debye temperature from the Lindemann'sproportional. According to this, a crystal will melt when the root mean square displacement of an atom exceeds a certain fraction of the interatomic distance in the crystal [11]. Connecting the specific heat theory with the Lindemann's melting formula; the characteristic temperature square is proportional to the melting point of the crystal. So, the Debye temperature for the bulk material is inscribed as [12]

$$\theta_{Db}^{\ 2} \propto \left(\frac{T_b}{MV^{2/3}}\right), \qquad (3)$$

Evenly for nanomaterial

$$\theta_{Dp}^{\ 2} \propto \left(\frac{T_p}{MV^{2/3}}\right), \qquad (4)$$

Where, M is the molecular mass.

Equations (3) and (4) give the following relation, we acquire

$$\left(\frac{\theta_{Dp}^2}{\theta_{Db}^2}\right) = \frac{T_p}{T_b} \qquad (5)$$

Consequently, from Eq. (2) and (5) we obtain

$$\left(\frac{\theta_{Dp}}{\theta_{Db}}\right) = \left(1 - \frac{N}{2n}\right)^{1/2} \qquad (6),$$

The technique to find $N/2n$ for different shape of nanomaterials has been debated by Qi [10]. The value of $\frac{N}{n}$ is $\frac{4d}{D}, \frac{8d}{3l}$ and $\frac{4d}{3h}$ for spherical nanosolids, nanowires and nanofilms respectively [10]. Where, d is the diameter of atom and D is the diameter of the spherical nanosolids. Here, l is the diameter of nanowire and h is the height of the nanofilm.

Table1. Input parameters used in present work [13, 14, 15]

Nanomaterials	Debye Temperature($\theta_{Db}(K)$	Atomic Size d(nm)
Au	165	0.2884
Cu		0.256

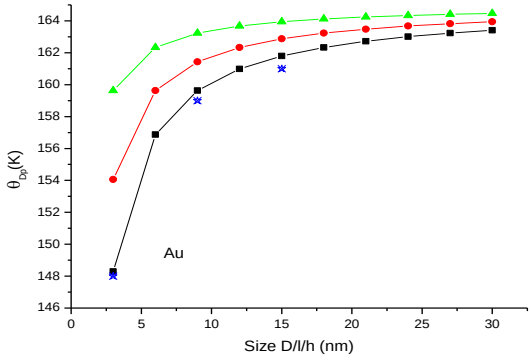

Fig. 1. Size dependence Debye temperature θ_{Dp} of Au (nanosphere, nanowire and nanofilm) calculated from Eq. (6). The lines with Symbols square, circle and triangle are for nanosphere, nanowire and nanofilm respectively. Experimental values for nanosphere are shown by stars [16].

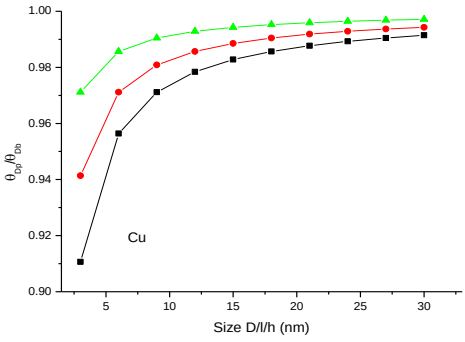

Fig. 2. Size dependence θ_{Dp}/θ_{Db} of Cu (nanosphere, nanowire and nanofilm) calculated from Eq. (6). The lines with Symbols square, circle and triangle are for nanosphere, nanowire and nanofilm respectively

II. RESULTS AND DISCUSSION

It is shown by Eq. (6) that the Debye temperature is the function of particle size and the shape of the nanomaterials. So, we can discuss the Debye temperature variation with the size of the particles and shapes of the materials. The variation tendency of the relative Debye temperature with respect to particle size and shape of nanomaterials calculated by Eq. (6) is shown in Fig. 1 and 2. Input parameters in our calculation are recorded in Table 1[13-15]. The variation of Debye temperature with particle size and shape of Au nanomaterial calculated from Eq. (6) is shown in Fig. 2 along with the available experimental values for Au nanosphere [16], which support well to our calculated results. This added the validity of the modelused. For the comparison purpose we have plotted the nanosphere, nanowire and nanofilm on the same Fig 1. It is observed that the effect of size decrease as we go from spherical to nanowire to nanofilm. The size and shape dependent Debye temperature of Cu nanomaterial computed using Eq. (6) is shown in fig 2. As exposed in figure, the Debye temperature goes down with the decrease of the particle size. For the sake of comparison, we plotted nanosphere, nanowire and nanofilm materials on the same graph. It is shown that on decreasing the particle size Debye temperature decreases more in spherical nanosolid in comparison to nanowire and nanofilmFor Cu nanomaterial, experimental values are not available. The main reason for the size dependent Debye temperature of nanomaterials is observed as the presence of the large fraction of surface atoms. When size decreases the surface to volume ratio increases, which increases the surface energy. Therefore, the value of $N/2n$ increases. Since the values of $N/2n$ are $\frac{2d}{D}, \frac{4d}{3l}$ and $\frac{2d}{3h}$. On decreasing D, l, h the factor $N/2n$ increases, accordingly the Debye temperature decreases and its effect is more on nanosphere and decreases from nanowire to nanofilm. These results may be of great attention of researches engaged in the experimentalreports.

III. CONCLUSION

We have examined a simple theoretical method to study the size dependence Debye temperature of nanomaterials in different shapes like nanosphere, nanowire and nanofilm. It is shown that the calculated results of Debye temperature of Au and Cu nanomaterials are consistent with the existing experimental results. Moreover, it is also realized that the particle shape effect the Debye temperature of the nanomaterials. The effect on Debye temperature becomes more with the reducing of particle size. Due to the simple process and the applicability of the model, theory may be extended to range of nanomaterials.

REFERENCES

[1] R Lamber, S Wetjen, I Jaeger,Size dependence of the lattice parameter of small palladium particles, Phys Rev B, 1995, 51,10968.
[2] H. Gleiter, Nanostructured materials: Basic concepts and microstructure, Acta Materialia, 2000, 48 1–29.
[3] T. Chookajorn, H.A. Murdoch, C.A. Schuh, Science 2012, 337, 951–954.
[4] S F Xiao, W Y Hu, J Y Yang, J Phys Chem B, 2005, 109, 20339.
[5] H K Kim, S H Hu, J W Park, J W Jeong, G H Lee, Chem, Phys Let, 354, 2002, 165-172.
[6] M Hou, M E Azzaoui, H Pattyn H, J Verheyden, G Koops, G Zhang, Phys Rev B, 2000, 62, 5117
[7] L H Liang, J C Li, Q Jiang, Solid state Communi, 2002, 121, 453.

[8] X W Wang, G T Fei, K Zheng, Z Jin, L D Zhang, Applied Phys Lett, 2006, 88, 173114.

[9] M Cottie, The weired world of nanoscale, University of Technology, Sydney, P O Box 123, Broadway NSW, Australia, 2007.

[10] W.H.Qi, Size effect on melting temperature of nanosolids Physical B, 2005, 368, 46.

[11] F.A. Lindemann, the Calculation of Molecular Vibration Frequencies, Phys. Z, 1910, 11, 609.

[12] J.G. Das, History of the search for continuous melting, Rev. Mod. Phys., 1999, 71, 1737.

[13] H.W. King, R.W.Cahn (Ed.), Physical Metallurgy, North Holland, Amsterdam, 1970.

[14] G. Kastle, H. G. Boyen, A. Shroder, A. Plettl, P. Ziemann, Phys. Rev. B, 2004, 70, 165414.

[15] HLiang, MUpmanyu, H Huana, Phys Rev B, 2005, 71, 241401.

[16] A. Balerna, S. Mobilio,Dynamic properties and Debye temperatures of bulk Au and Au clusters studied using extended x-ray-absorption fine-structure spectroscopy, Phys. Rev. B Condens. Matter, 1986, 34, 2293.