



Study of Size Dependent Thermal Conductivity of Gold FCC Nanomaterial

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Abstract: A theoretical model for the study of size dependent thermal conductivity of Gold FCC nanomaterial has been developed by considering the cluster order with particle size of Gold (Au) FCC nanomaterial. Using this model, the thermal conductivity of Gold FCC nanomaterial has been calculated and compared with other theoretical models and existing experimental data. It is found that the thermal conductivity of Gold FCC nanomaterial decreases as the size of the nanoparticle decreases. The comparison of theoretical findings of the present work indicates that the developed theoretical model is in good agreement with available experimental data which shows the validity of the present work.

Keywords: size, thermal conductivity, gold, nanomaterial

I. Introduction

The physical properties of nanomaterials have been investigated extensively both theoretically and experimentally due to their scientific and industrial importance [1]. It has been reported that the nanomaterials exhibit interesting physical, chemical, electrical and thermal properties that are significantly different from the corresponding properties of bulk materials [2-4]. Because of the enormous surface area to volume ratio of nanomaterials, the energy associated with the atoms of these nanomaterials will be different in comparison of conventional bulk materials, leading to the size dependent properties of nanomaterials[5]. The energy of the free surface atoms is entirely different as compared to the energy related to the atom of the bulk. The surplus energy associated with the surface atom is known as the free surface energy. In bulk materials, this free surface energy is neglected because it has associated with only top most layers of the atoms on the surface. Also the ratio of the resided volume of surface atoms and the total volume of the material is extremely small.

As the size of the low dimensional materials decreases to the nanometer size range, the electronic, magnetic, optic, catalytic, electrical and thermal properties of these materials are significantly altered from those of either the bulk or a single molecule [1]. Among these properties, the thermal conductivity of nanomaterials have received considerable attention because thermal conductivity is a fundamental property of nanosolids that directly affects its applications. However, few efforts have been focused on studying thermal conductivity of these materials.

Some experimental studies have been carried out to investigate the effect of nanoparticles on the thermal conductivity of various materials. Katika and Pilon [6] have studied the effect of size of nanoparticles on the thermal conductivity of crystalline thin films at low temperatures and reported that the thermal conductivity decreases with decreasing particle radius. There are some theoretical studies on the size effect on thermal conductivity of nanomaterials. Singh et al. [7] have studied the grain-size effect on the thermal conductivity of nanosolids and found that the thermal conductivity of nanosolids decreases as the grain size decreases. Very recently, Bhatt et al. [8] have proposed a theoretical model to study the size effects on thermal conductivity of nanomaterials and found a significant reduction in the thermal conductivity of nanomaterials by decreasing the size. Li et al. [9] have reported the decrease in thermal conductivity of nickel nanoparticles with decrease in their size. It is found that very few experimental and theoretical works have been done in this field while sufficient work is required in this direction. In all these studies, the crystal order of the materials has not been taken into account as it plays a vital role in the study of thermal conductivity of various nanomaterials. When the concentration of building blocks (atoms or ions) of a solid becomes enough high, they accumulate into small clusters through homogeneous nucleation. With continuous supply of the building blocks, these clusters tend to coalesce and grow to form a large cluster assembly. The cluster may be considered as an onion-like structure formed by many concentric shells around the central site. All surface site, which may belong to various shells, are defined as crusts, the number of crusts, n , defines the order of the cluster [9, 10]. It is, therefore, interesting to study and analyze the size effect on thermal conductivity of nanomaterial by considering the effect of cluster order. In the present work, we have modified available theoretical model by including cluster order for the study of thermal conductivity of Gold FCC nanomaterials.

II. Theoretical Model

The thermal conductivity of a nanomaterial is given as [7, 13]-

$$K_n = K_b \left(1 - \frac{N_s}{2N}\right)^{\frac{3}{2}} \quad \dots(1)$$

Where K_n , K_b , N_s and N are thermal conductivity of nanomaterial, thermal conductivity of bulk material, number of surface atoms and total number of atoms in the nanosolid. The value of $\frac{N_s}{2N}$ depends upon the structure of the nanomaterial and is different for different shape of nanomaterials.

The surface – to- volume ratio $\frac{N_s}{N}$ for FCC structure as a function of cluster order ‘n’ is given as [9]-

$$\frac{N_s}{N} = \frac{30n^2+6}{10n^3+15n^2+11n+3} \quad \dots(2)$$

But cluster order ‘n’ is given as [9]-

$$n = \frac{1}{2} \left(\frac{r}{r_0} - 1 \right) \quad \dots(3)$$

where ‘r’ and ‘ r_0 ’ are the particle size and atomic radius of nanoparticles.

From equations (2) and (3), we get-

$$\frac{N_s}{N} = \frac{30\left(\frac{r}{r_0}-1\right)^2+24}{\left(\frac{r}{r_0}\right)\left[5\left(\frac{r}{r_0}\right)^2+7\right]} \quad \dots(4)$$

The above equation can be written in terms of diameter ‘D’ as-

$$\frac{N_s}{N} = \frac{30\left(\frac{D}{d}-1\right)^2+24}{\left(\frac{D}{d}\right)\left[5\left(\frac{D}{d}\right)^2+7\right]} \quad \dots(5)$$

(Since $r_0 = \frac{d}{2}$ and $r = \frac{D}{2}$)

Where ‘d’ and ‘D’ are atomic diameter and particle diameter.

Therefore, equation (1) takes the form as-

$$K_n = K_b \left[1 - \frac{15\left(\frac{D}{d}-1\right)^2+12}{\left(\frac{D}{d}\right)\left[5\left(\frac{D}{d}\right)^2+7\right]} \right]^{\frac{3}{2}} \quad \dots(6)$$

Equation (6) is the modified equation for thermal conductivity of nanomaterials which has been derived by including the effect of cluster order ‘n’ in terms of the size of the nanomaterials. Using this equation, we can study the size dependence of thermal conductivity of FCC nanomaterials.

III. Results and Discussion

The equation (6) is the modified equation which can be used to study size dependence of thermal conductivity of nanomaterials. The nanomaterials can have different geometrical shapes such as cubo-octahedral (co), icosahedra (ico), body centred cubic (bcc) and simple cubic (sc). Clusters with a small number of atoms crystallize in the form of ico. The structure becomes unstable for a large number of atoms and transforms to co which is just a patch of the face centred cubic (fcc) [9]. In the present work, using equation (6), we have calculated the thermal conductivity of Gold FCC nanomaterial with their size. The unique properties of Gold at the nanoscale lead to its use in a growing number of applications including colloids for biomedical marking and catalysts in chemical processing and pollution control. For Gold, the values of atomic diameter ‘d’ is 0.288 nm [7] while the thermal conductivity for Gold bulk material ‘ K_b ’ is 315 Wm⁻¹K⁻¹ [11]. These parameters are used as input parameters in computational work. The calculated theoretical values of thermal conductivity of Gold FCC nanomaterial are plotted against the varying particle size in figure (1). From the figure, we can see that the thermal conductivity of Gold FCC nanomaterial decreases as the size of nanoparticle decreases. For the size larger than 20 nm, the thermal conductivity becomes almost constant as the figure shows, The observed drift is predictable due to the increase in the surface-to-volume ratio as the nanoparticle size is decreased. Because of lower coordination of the atoms near the surface induces a corresponding rearrangement of the electric charge and the binding state changes [12]. Therefore, the cohesive energy of these atoms will vary from that of its bulk counterpart. Therefore, the thermal conductivity of the free surface region differs from that of the bulk material. Theoretically obtained results are compared with the available experimental data and theoretical results. Our theoretically obtained results are very close to the experimental results that confirms the validity of our work.

IV. Conclusion

In conclusion, we have developed a theoretical model to understand the effect of size of nanoparticle on thermal conductivity of Gold FCC nanomaterial by considering the cluster order. The calculated theoretical values of thermal conductivity of Gold FCC nanomaterial are plotted against the varying particle size and found a significant reduction in the thermal conductivity of Gold FCC nanomaterial with decrease the particle size. Theoretically

obtained results are compared with the available experimental data and theoretical results. The comparison shows that our results are in excellent agreement with other reported works which shows the validity of the present work.

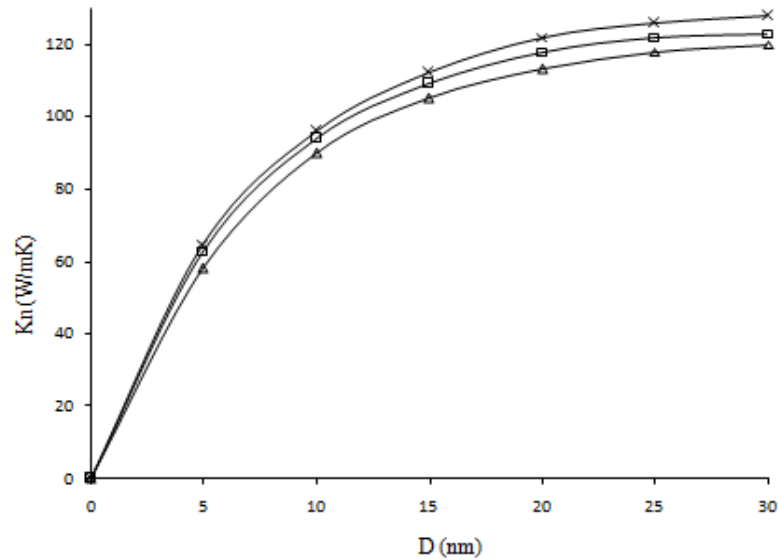


Figure (1): Size dependent thermal conductivity of Gold FCC nanomaterial shown using square were obtained from equation(6). Experimental values are shown by cross [11] while other theoretical results[7] are shown by triangle.

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