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Effects of *Grain-Size* on Debye Temperature and Thermal Conductivity of Nanomaterials

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Abstract
A hypothetical model is accounted for to compute the warm conductivity of nanomaterials in various shapes, for example, round nanosolids, nanowires and nanofilms dependent on size subordinate nuclear strong energy on thinking about the surface impacts. It is seen that the warm conductivity of various shapes nanosolids diminishes with decline in the grain size. The outcomes acquired are contrasted and the accessible test information. A nearby arrangement among hypothesis and investigation support the legitimacy of the strategy talked about.
Keywords: *grain-size, nanomaterials*

I. Introduction

Nanomaterials are establishments of nanoscience and nanotechnology. The possibility of nanotechnology felt without precedent for the renowned talk " There is a lot of room at the base" given by the Physicist Richard Feynman at the American Physical Society meeting on December 29, 1959 at Caltech. Nanostructure science and innovation is a wide and interdisciplinary dynamic space of innovative work interest that has been sustaining worldwide in the beyond couple of years. Nanomaterials are energizing since they show solid shape and size impacts, which can't be clarified by standard hypotheses. Nanocrystals have huge surface-to-volume proportions, and surface impacts take on an importance that is regularly irrelevant for mass materials. At nanoscale Au and Ag have exhibited many intriguing substance and actual properties that can't be seen from their mass partners [1-3]. Liu et al. [4] fostered a model to accommodate the noticed size reliance of grid strain, center level shift and versatile modulus of Au and Ag nanostructures which depends on Goldschmidt Pauling's standard of bond compression and its expansion to the neighborhood bond energy and restricting energy thickness. Different models, for example, surface strain; surface unwinding, surface pressure, grid vibration precariousness and surface phonon unsteadiness have been created to comprehend the surprising practices of metallic nanostructures [5-9]. A bound together insightful model with regards to the size subordinate versatile modulus and vibration recurrence of nanocrystalline metals, earthenware production and semiconductors is set up dependent on the intrinsic cross section strain and the limiting energy change of nanocrystals [10]. Additionally, the hypothetical clarification for the size impact of the versatile modulus [11] and volume warm extension [12] are connected with the surface impact by presenting the surface energy commitment.

Free surface Atoms encounters a not at all like nearby climate than do particles in the majority of a materials. As an outcome, the energy related with these molecules will be not the same as that of the iotas in the mass. The additional energy imparted to surface molecules is known as the surface energy. Surface free energy is typically ignored in regular continuum mechanics, since it is related with a couple of layers of molecules close to the surface and the proportion of the volume involved by the surface iotas and the absolute volume of the material of interest is minuscule. The investigation of size and shape consequences for nanomaterials has drawn in gigantic consideration because of their logical and modern significance. Warm conductivity is the key properties of nanosolids, which tells straightforwardly to its application. Nonetheless, not many endeavors have been executed for the warm conductivity. In this paper, on considering the surface impacts, we present another model to compute the warm conductivity of nanosized Si, GaAs, Sn, Ag, and Au and in underlying (round nanosolids, nanofilms and nanowires) nonmaterial depends on size subordinate nuclear strong energy. The model expectations concur well with the accessible trial results.

II. Method Of Analysis

The amount of energy because of the commitments of the inside iotas and the surface molecules of the nanomaterials is characterized as durable energy, which is communicated as [13]

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

Where n is the total number of atoms of nanosolids and the number of its surface atoms is N. Therefore, $(n-N)$ is the absolute number of insides molecules of the nanomaterials. E0 is the firm energy of the mass materials per molecule. Eq. (1) might be composed as

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

Where E_p is the cohesive energy per mole of the nanomaterials, which is given by $\frac{AE_{sum}}{n}$ Here, A is the Avogadro constant. Eb is defined as the cohesive energy per mole of the corresponding bulk materials which is given by $E_b = AE_0$. Qi [13] reported the relation between the melting point of nanomaterials and bulk as:

$$T_p = T_b\left(1-\frac{N}{2n}\right) \qquad (2)$$

Thermal conductivity k of bulk materials is expressed as [14]

$$k_b = (1/3)cv_b l_b, \qquad (3)$$

Here, c is the particular hotness, b v the normal phonon speed and b l is sans mean way. Warm conductivity relies on explicit hotness, normal phonon speed and mean free way. At room temperature, we accepted explicit hotness is steady. We think about the size reliance of p v and p l for the warm conductivity of nonmaterial's. Likewise, we write thermal conductivity for nanomaterial as

$$k_p = (1/3)cv_p l_p \qquad (4)$$

Combining (3) and (4), we get the following relation:

$$\frac{k_p}{k_b} = \left(\frac{v_p l_p}{v_b l_b}\right) \qquad (5)$$

The Debye temperature is proportional to average phonon velocity of the crystal [17] written as, $\theta_b \propto \frac{2h}{\pi k_B}\left(\frac{3N_A}{4\pi V}\right)^{1/3} v_b$ (6)

Likewise, we can write for nanomaterials:

$$\theta_p \propto \frac{2h}{\pi k_B}\left(\frac{3N_A}{4\pi V}\right)^{1/3} v_p \qquad (7)$$

Where, h the Planck constant, NA the Avogadro number, Boltzmann constant B k , and the molar volume are. Combining equation (6) and (7) gives the following relation:

$$\frac{v_p}{v_b} = \frac{\theta_p}{\theta_b}, \qquad (8)$$

One might get the connection between the softening point and the Debye temperature from the Lindemann's corresponding. As per this a precious stone will soften when the root mean square relocation of a particle surpasses a specific part of the interatomic distance in the gem. Joining the particular hotness hypothesis with the Lindemann's softening recipe; the trademark temperature square is corresponding to the dissolving point of the precious stone. In this way, the Debye temperature for the mass material is composed as

$$\theta_b^{\,2} \propto \left(\frac{T_b}{MV^{2/3}}\right), \qquad (9)$$

Likewise for nanomaterial

$$\theta_p^{\,2} \propto \left(\frac{T_p}{MV^{2/3}}\right), \qquad (10)$$

Where, M is the molecular mass. Equation (9) and (10) give the following relation:

$$\left(\frac{\theta_p^2}{\theta_b^2}\right)=\frac{T_p}{T_b}$$

$$\text{Or, } \left(\frac{\theta_p}{\theta_b}\right)=\left(1-\frac{N}{2n}\right)^{1/2} \qquad (11),$$

Ling and Li [20] reported the following relation for the mean free path:

$$\left(\frac{l_p}{l_b}\right)=\frac{T_p}{T_b} \qquad (12),$$

Therefore, putting the value of Eqs. (8-11), in Eq. (5), we get the Following relation:

$$k_p = k_b\left(\frac{T_p}{T_b}\right)^{3/2}, \quad (13)$$

Thus, from Eq (2) and (13), we get the final relation for thermal conductivity of nanomaterials as follows:

$$k_p = k_b\left(1-\frac{N}{2n}\right) \quad (14),$$

The value of $\frac{N}{n}$ is $\frac{4d}{D}, \frac{8d}{3l}$ and $\frac{4d}{3h}$ for circular nanosolids, nanowires and nanofilms separately Where, d is the width of nanosolid and D is the measurement of the circular nanosolids. l and h are the width of nanowire and stature of the nanofilm separately

Table 1. Input parameters used in theoretical calculations [21, 22, 23]

	Si	GaAs	Sn	Ag	In	Au
d(nm)	0.336	0.245	0.376	0.289	0.329	0.288
$\theta_{b\,(K)}$				225		165

III. Results and Discussion

We set up a straightforward hypothetical model to concentrate on the impact of size on the warm conductivity of various states of nanosolids. The info boundaries d and (Debye temperature) needed in hypothetical estimations are recorded in Table 1. To check the legitimacy of our model we likewise determined the Debye temperature of Au and Ag nanosolids. The Debye temperature unequivocally relies on the design of the materials. It is likewise straightforwardly identified with the limiting power between the molecules Besides, Debye temperature is the essential information to comprehend the thermodynamical properties like Helmholtz free energy, cross section vibration [8], explicit hotness limit and warm conductivity. Utilizing the peculiarity of iota vibration, proposed the hypothesis to talk about the Debye temperature of mass materials by this

$$\theta_p^{\,2} \propto \left(\frac{T_p}{MV^{2/3}}\right)$$

Connection. We utilized Eq. (11) to anticipate the grain size subordinate Debye temperature of Au and Ag nanosolids. The outcomes got are communicated in figure 1. It is observed that the Debye temperature diminishes with decline in grain size. The Experimental qualities are accessible for Au which has been included for the correlation reasons. It is seen that the model forecasts are as per the test realities. We have stretched out this hypothesis to ascertain the warm conductivity of nanosized Si, GaAs, Sn, Ag, and Au and In underlying (circular nanosolids, nanofilms and nanowires) nanomaterials, in light of the way that some test information are accessible so the model can be checked by examination. The outcomes got are displayed in figs. 2-7, with accessible exploratory information for correlation. The grain size subordinate warm conductivity of Si nanofilm registered utilizing Eq. (14) is accounted for in Fig. 2 alongside the accessible exploratory information for correlation reason. The qualities determined by our model can be seen to nearer to the accessible exploratory qualities It is seen that warm conductivity diminishes with diminishing the grain size. This uncovers the

reasonableness of the plan utilized. From Fig 7., it is seen that the warm conductivity variety with size of In is extremely near Si, Sn and GaAs. It is a direct result of the way that, the warm conductivity of in mass is 81.8 w/m/s, which is extremely near the warm conductivity of Sn (68W/m/s), GaAs (55 W/m/s) and Si (149 W/m/s). Though, the warm conductivity of Ag and Au in mass are 429 w/m/s and 318 W/m/s separately It ought to be referenced that the trial esteems are not accessible for the others nanomaterials, GaAs, Sn, Ag, Au and in viewed as in this paper. We are enrolling our model forecasts in the absence of trial esteems. These forecasts might be of current significance to the researchers occupied with the trial investigations. We have determined the grain size reliance of warm conductivity of GaAs, Sn, Ag, Au and In nanomaterials in various shapes like circular nanosolids, nanofilms and nanowires and detailed in the relating figures for correlation.

The qualities procured are expressed in Figs. 2-7. This float is unsurprising in light of the fact that the surface to volume proportion increments with diminishing size. Eq. (14) size subordinate warm conductivity of the nanosolids is gotten from their grain size subordinate strong energy. Since then brought down coordination of molecules close to the surface initiates a relating revamp of electric charge, which changes the limiting state.As an outcome, the firm energy of these particles will change from that of its mass partners. Hence, the warm conductivity of the free surface area contrasts from the mass materials. The impact of size diminishes as we go from round to nanowire and nanofilm. At the point when, we look at N/2n for circular to nanowire to nanofilm, the proportion becomes 3:2:1. Thusly, the warm conductivity variety for round nanoparticle, nanowire and nanofilm become 3:2:1 for a similar grain size. By this model, we concentrate on the impacts of surface free energy on the warm conductivity of nanosolids, nanowires and nanofilms.

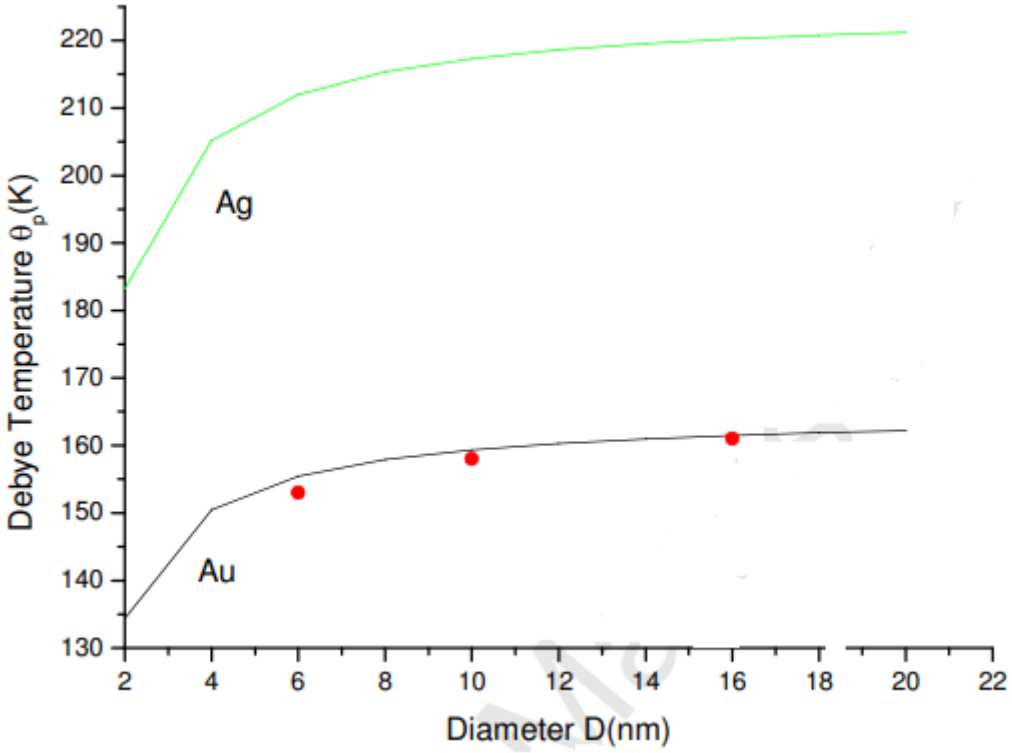

Fig. 1. Grain size dependent Debye Temperature of Au nanosolid and Ag nanosolid shown by solid lines using Eq. (11) Experimental values are shown by the solid circles for Au [25].

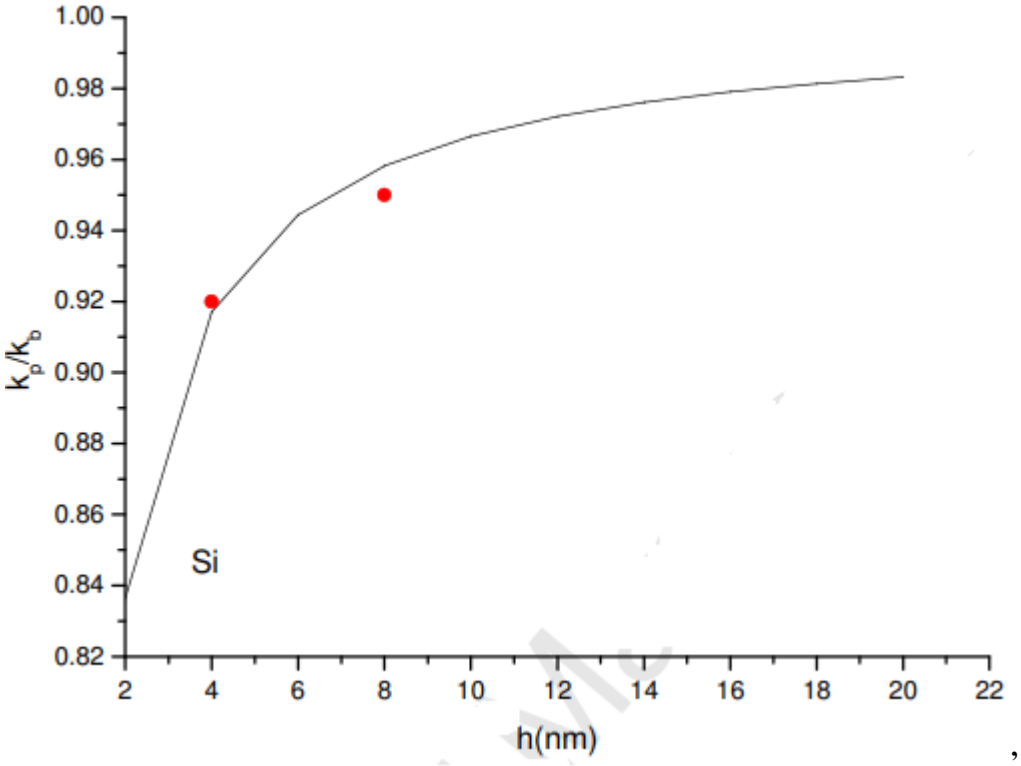

Fig. 2. Grain size dependent thermal conductivity of Si film (solid line) from our model in terms of Eq. (14).The symbol solid circles shows the experimental values [26]

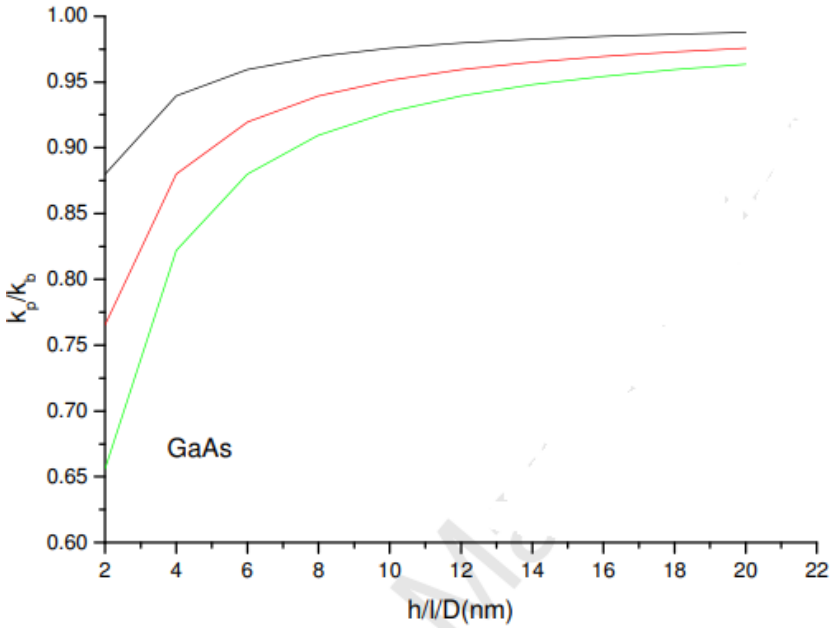

Fig. 3. Grain size dependent thermal conductivity of GaAs (spherical nanosolids, nanowires and nanofilms) bottom to top (green, red and black lines) from our model in terms of Eq. (14).

IV. Conclusions

In summary, a model for size subordinate the warm conductivity of nanomaterials is set up subject to Lindemann's premise and the surface effects. It is shown that the warm conductivity of Si, GaAs, Sn, Ag, Au and in nanosolids, nanofilms and nanowires decreases with decrease in grain size. We are sure that the current model may be of likely application in the investigation where, exploratory data is lacking.

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