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The Debye Temperature of Metallic Nanoparticles

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Abstract
Expectations for the variety of actual properties of nanomaterials have involved incredible discussion in late many years. Various specialists have announced uncommon changes in the actual properties of metals at their nanoscale. In the current work, we have concentrated on the Debye temperature of round nano strong, nanowire and nanofilms of Aluminum (Al), Copper (Cu), Palladium (Pd), and Platinum (Pt) having their sizes under 30 nm. For calculation, we have thought about the central connection of durable energy with a softening point. During our review, it is found that there is an uncommon change in the Debye temperature of round nano strong, nanowire and nanofilms of metals under 20 nm. In this variation,it is additionally seen that there is a greatest variety of Debye temperature is on account of nanofilms while least on account of circular nano solids and moderate change on account of nanowires. Variety in Debye temperature has been deciphered based on the presence of various surface molecules because of the adjustment of surface to volume proportion of metals at the nano level. We have contrasted our processed outcomes and the accessible test information which shows their great understanding.
Keywords: *Debye, Nanoparticles*

I. Introduction:

In the nanoscience and nanotechnology, the size of materials has diminished at the exceptionally low scope nanometer no less than one aspect. In this size range, the surface to volume proportion is quite expanded and correspondingly the physical, synthetic, and mechanical properties are changed [1-3]. The properties of material at nanoscale are unique in relation to the comparing mass material. The property of nanomaterials change definitely as the size decreases less than 30 nanometers.A test of gold seems red at 10 nanometers Its liquefying temperature diminishes quickly as their sizesare decreased up to the degree of nano scale [4-5]. Our motivation is to decide the Debye temperature of the nanomaterials which is firmly identified with the durable energy of the nanomaterials. The durable energy or hotness of sublimation is a significant actual amount to represent the strength of metallic bonds. The firm energy is the energy to partition the metallic gem into individual particles. For the above said reason we concentrated on the situation of state for the size subordinate Debye temperature of the nanoparticles of metals Aluminum (Al), Copper (Cu), Paladium (Pd) and Platinum (Pt). We have processed the Debye temperature of circular nanosolid, nanowire and nanofilm of the thought about examples. With the diverse method of variety, it is seen that the Debye temperature of metals at nano levelincreases with increment of theirsizes.

II. Method Of Analysis:

The total cohesive energy of the nano crystalline solid, is given by

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

Condition (1) is the amount of energy because of the commitment of the inside molecules just as the surface iotas of nanocrystalline solids. Here $E0$ is the durable energy of the mass materials per molecule, n is the all out no of iotas of nano strong and N is the quantity of particles at the surface. [6]
For the cohesive energy per mole, the equation (1) may be written as

$$A_vE_{tot} = E_0A_v\,(n-N) + \frac{1}{2}A_vE_oN$$

$$\frac{A_vE_{tot}}{n} = E_0A_v\left(1-\frac{N}{n}\right) + \frac{A_vE_0\,N}{2n} \ldots (2)$$

Where,v is Avagadro number. The term $\frac{A_vE_{tot}}{} = En$represents the cohesive energy per mole of the nanocrystalline solid and $E_0A_v = E_b$ is the cohesive energy per mole of the corresponding bulk material.

Thus equation (2) becomes,

$$E_n = E_b(1 - \frac{N}{2n}) \ldots (3)$$

Since the strong energy is straightforwardly related to the melting temperature,[7-8], in this way the dissolving temperature of the nanosolid can be created as

$$T_{mn} = T_{mb}(1 - \frac{N}{2n}) \ldots (4)$$

According Lindermann criterion, a crystal melts when the root mean square displacement of atoms in the crystal exceeds a certain of the interatomic distance in the crystal[9]. The Debye temperatureθD is related with melting temperature as,

$$\theta_D = constt.\left(\frac{T_m}{MV^{2/3}}\right)^{1/2} \quad \ldots\ldots (5)$$

Where M is the molecular mass and V is the volume per atom.
If $\theta Dn$and θDb address the Debye temperature of material of nano estimated and of mass material individually, we can compose,

$$\frac{\theta_{Dn}}{\theta_{Db}} = \left(\frac{T_{mn}}{T_{mb}}\right)^{1/2} \quad \ldots\ldots\ldots (6)$$

$$\frac{\theta_{Dn}}{\theta_{Db}} = \left(1 - \frac{N}{2n}\right)^{1/2} \quad \ldots\ldots (7)$$

The value of $\left(\frac{N}{2n}\right)$ depends upon the structure of the nanomaterial and has been calculated for different shape of nanomaterials [5].

For spherical nanosolids, $\frac{N}{2n} = \frac{2d}{D}$ .....(8)
Where, D and dare the diameters of spherical nanosolid and that for atom respectively.

For nanowires, $\frac{N}{2n} = \frac{4d}{3L}$ .....(9)
Where, L is diameter of nanowire.

And for nanofilm, $\frac{N}{2n} = \frac{2d}{3h}$ .....(10)
Where h is height of nanofilm.

Table: 1: Input Parameters of Eq. (4) and Eq. (7)

Metals	Atomic Diameter, d (nm) .[11]
Copper (Cu)	0.2822
Palladium (Pd)	0.3040
Platinum(Pt)	0.3064
Aluminum (Al)	0.3165

III. Result And Discussion

In our current work we have concentrated on the variety of liquefying and Debye temperature of nanocrystalline metals given in the table-1. To figure the dissolving temperature of nanocrystalline copper, palladium, platinum and aluminum condition (4) is utilized in which the necessary info information has been taken from table-1 [3]. The figured benefits of liquefying point (temperature) of Cu, Pd, Pt and Al (nanosolid, nanowire and nanofilm) are plotted against the size of comparing nanostructures given in Fig.(1) – Fig.(4) alongside accessible exploratory data[10]. During our investigation of size reliance of softening temperature, it is found that liquefying temperature of metal nanostructures diminishes in the little scope of their sizes (10-20nm) later that it turns out to be practically consistent.

The liquefying bends can be isolated into two sections, sizes bigger than 10 nm and sizes under 10 nm. Softening temperature changes tenderly with the variety of size and the bends are almost even for D >10 nm.

However, the adjustment of dissolving temperature is a lot of quick under 10 nmin instances of these metallic nanostructuredmaterials. Again we can see that past 20 nm of the size of the material, the proportion of softening temperature at nanoscale to the mass turns out to be practically steady.

The widespread connection for size subordinate thermodynamic properties of metallic nanoparticles proposed by Xiong et al [6] likewise foresee similar size subordinate variety of dissolving point in the event of metals. Likewise the adjustment of liquefying temperature for nanosolids is bigger than that of nanowires and nanofilms. This is because of the quick expansion in surface to volume proportion at more modest nanoscale.Our processed outcomes are in great concurrence with the test information got by Buffat [11] and Shim[12] who estimated the liquefying temperatures utilizing the filtering electron diffraction and dissipation rate estimation methods, separately. An arrangement among hypothetical and test information urged us to stretch out this model to the Debye temperature. We have stretched out our review to the Debye temperature of these nanocrystalline structures. To concentrate on the size reliance of Debye temperature of chose tests we use condition (7) which is changed relating to the nanosolids, nanowires and nanofilms utilizing condition (8-10). The processed hypothetical upsides of Debye temperature of Cu, Pd, Pt and Al are plotted against the changing sizes of their nanostructures are displayed in Fig. (5)- Fig. (8). From these figures, we can see that Debye temperature diminishes with decline in size of nanomaterials yet this adjustment of Debye temperature is less fast than the liquefying temperature. This is on the grounds that the Debye temperature shifts as square base of liquefying temperature. For the size bigger than 20 nm, the proportion of Debye temperature at nanoscale to the mass material turns out to be practically steady, as displayed the charts. Like the variety of liquefying point with size the adjustment of Debye temperature for nanosolids is bigger than that of nanowires and nanofilms.

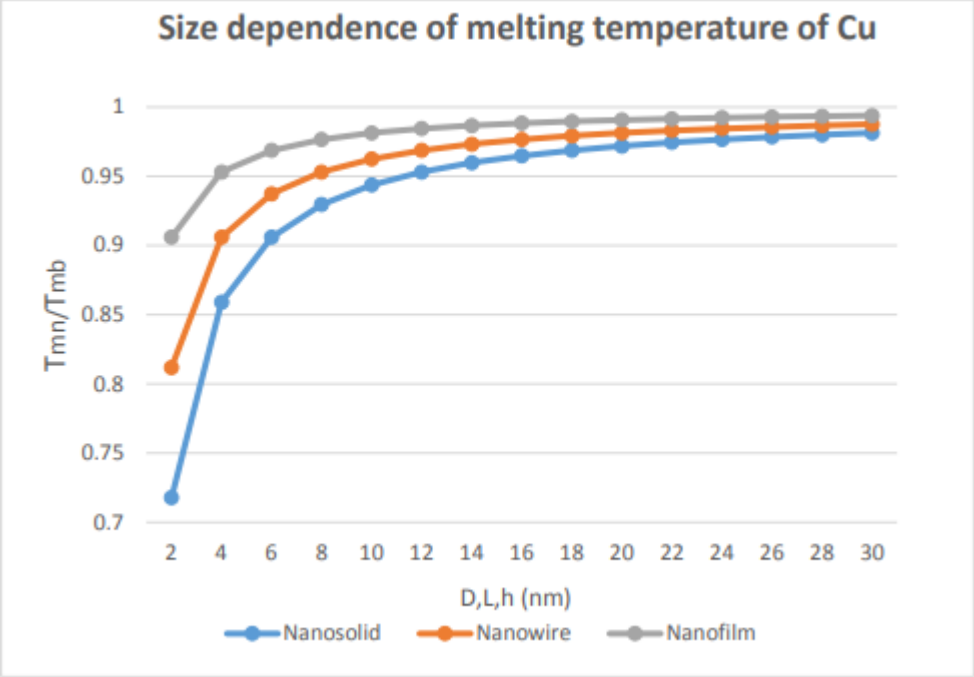

Fig. 1 Size dependence of melting point of nanocrystalline Copper (Cu)

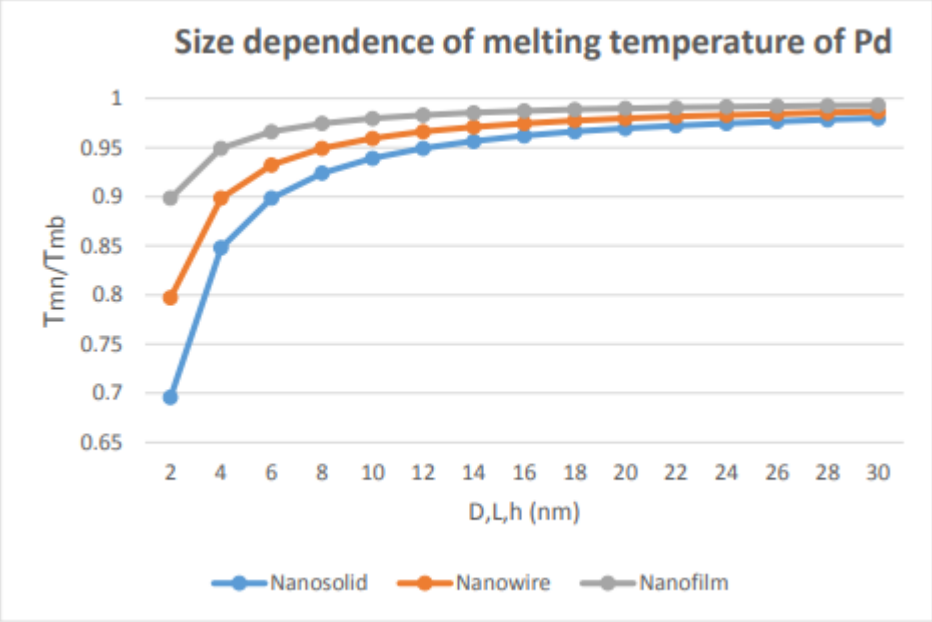

Fig. 2 Size dependence of melting point of nanocrystalline Palladium (Pd)

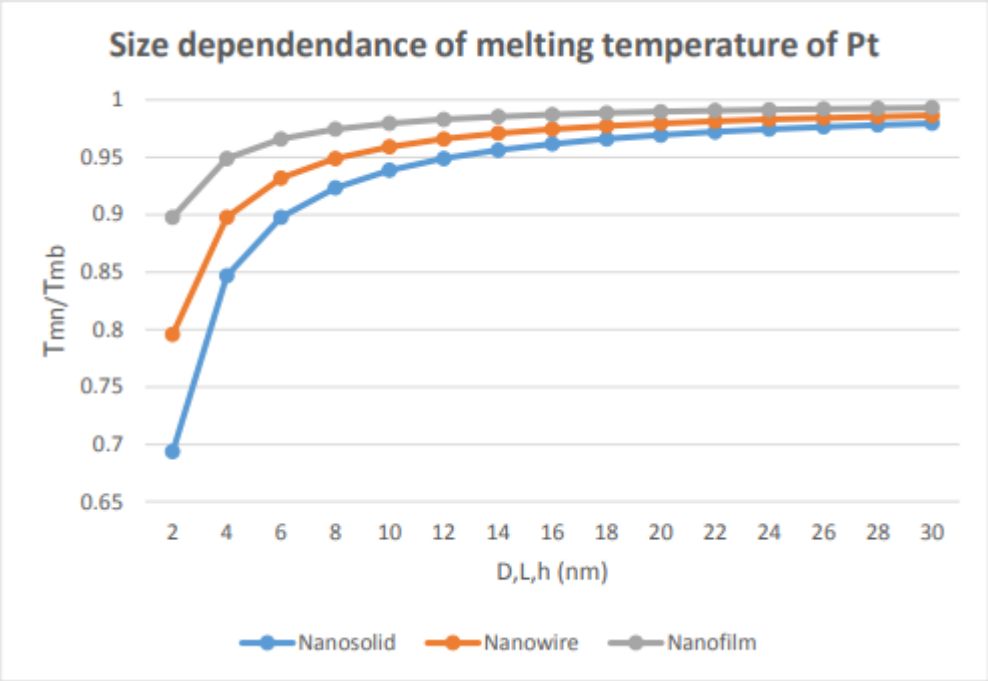

Fig.3 Size dependence of melting point of nanocrystalline Platinum (Pt)

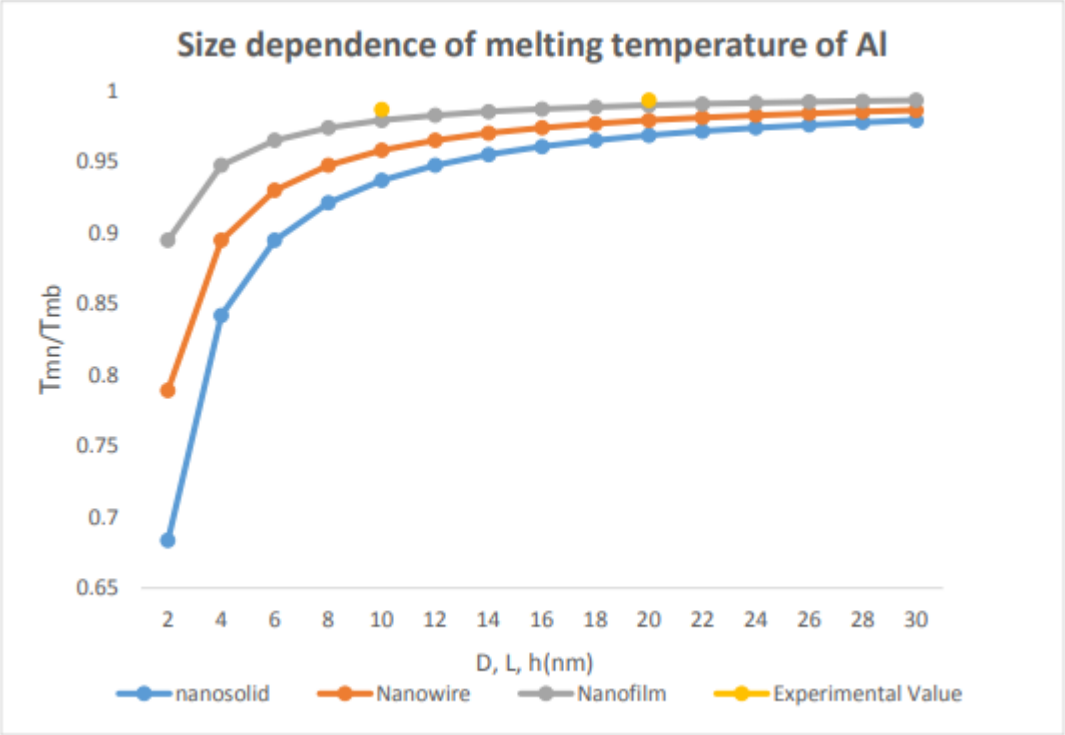

Fig. 4 Size dependence of melting point of nanocrystalline Aluminium (Al)

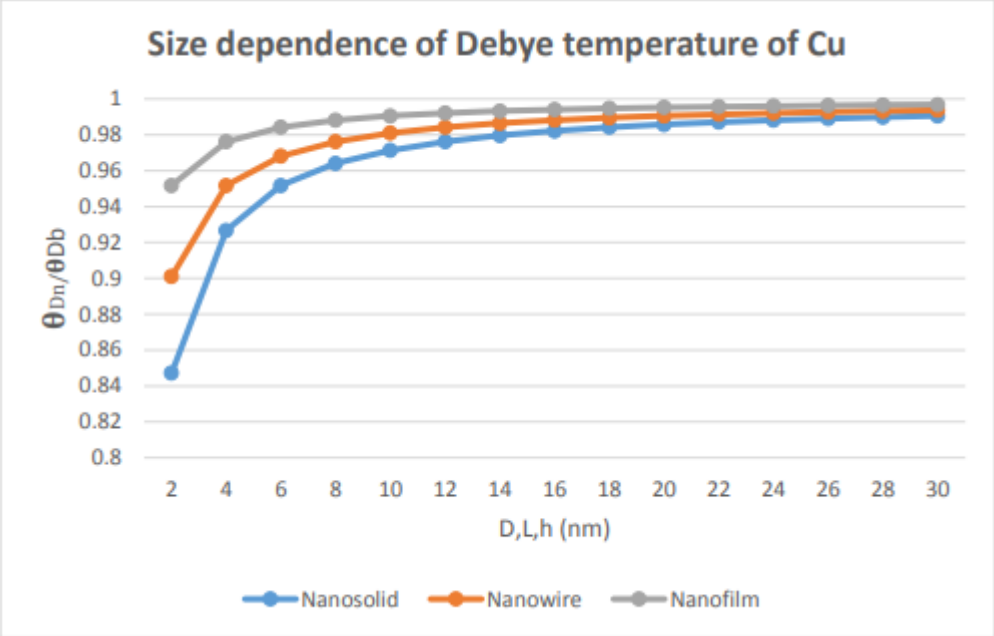

Fig. 5 Size dependence of Debye temperature of nanocrystalline Copper (Cu)

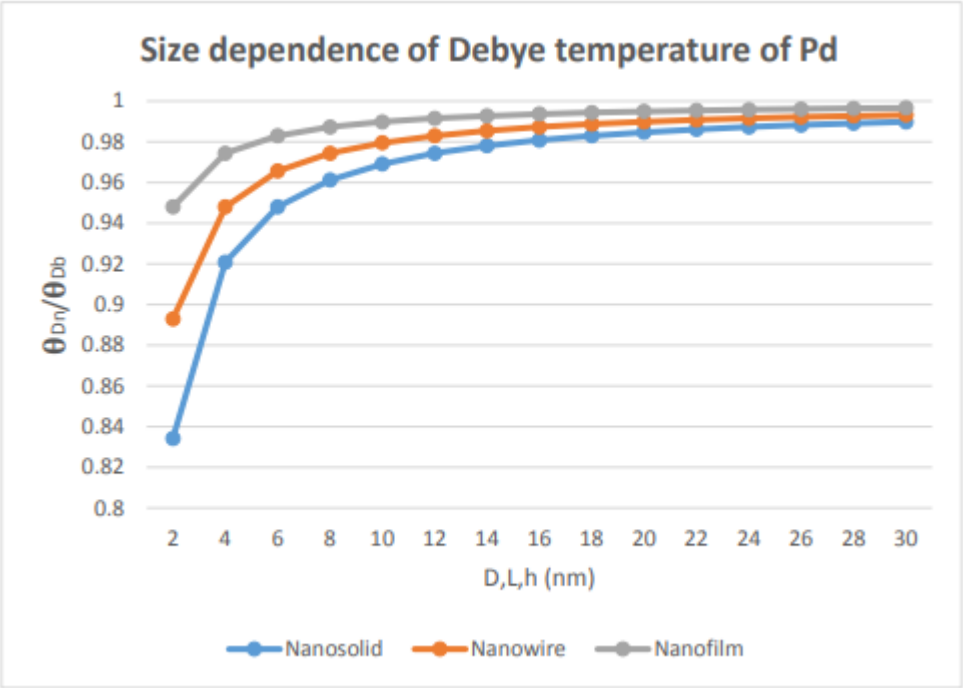

Fig. 6 Size dependence of Debye temperature of nanocrystalline Palladium (Pd)

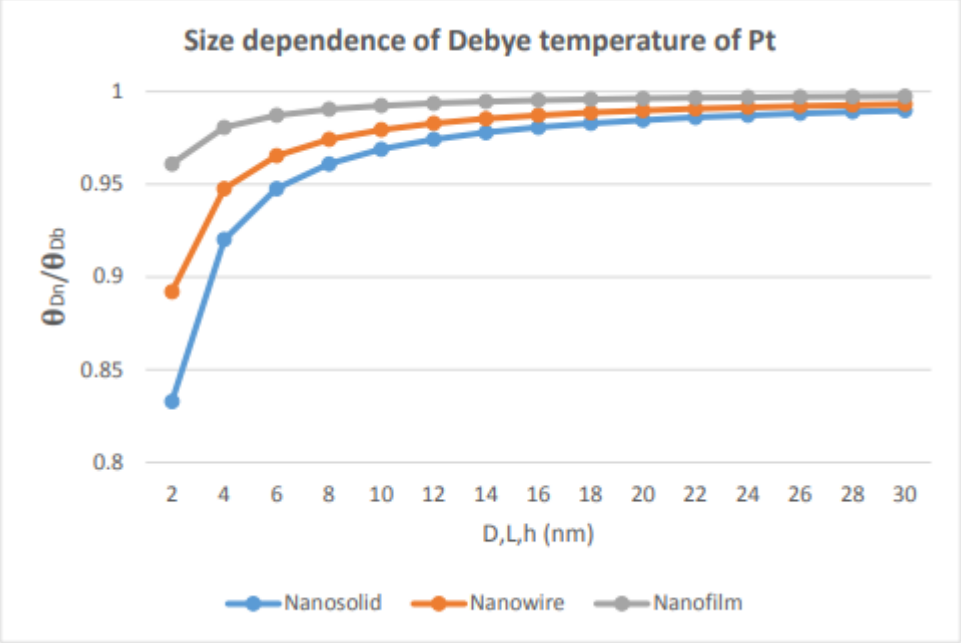

Fig. 7 Size dependence of Debye temperature of nanocrystalline Platinum (Pt)

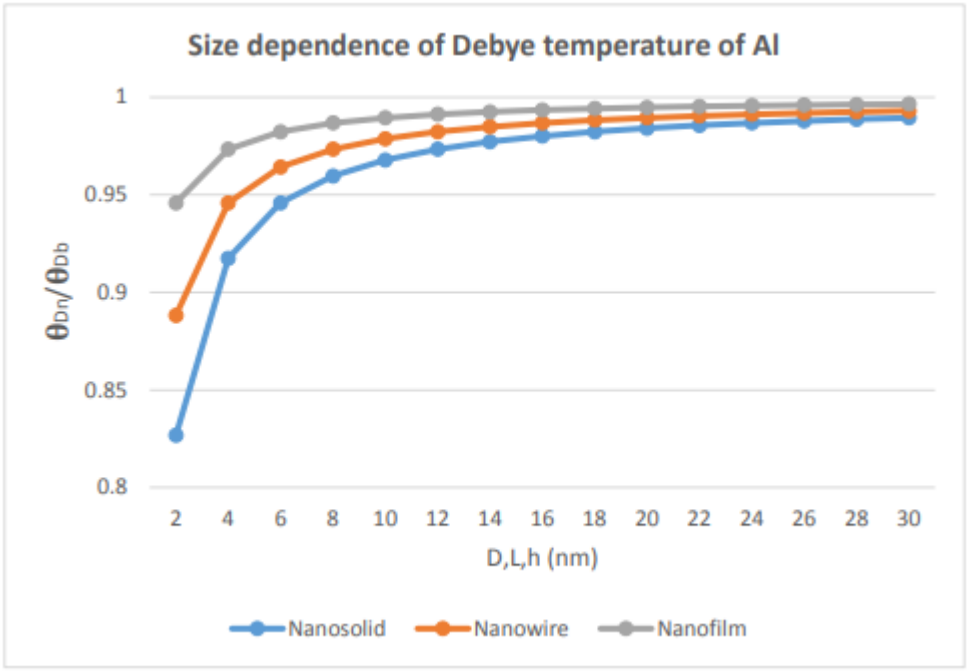

Fig. 8 Size dependence of Debye temperature of nanocrystalline Aluminum (Al)

IV. Conclusion:

If there should arise an occurrence of metallic nanostructured materials dissolving temperature changes delicately with the variety of size and the bends are almost flat for D >10 nm, which turns out to be especially conspicuous under 10 nm. Past 20 nm of the size of the material, the proportion of liquefying temperature at nanoscale to the mass turns out to be practically steady. The Debye temperature of metallic nanostructured materials additionally diminishes with decline in size of nanomaterials however this adjustment of Debye temperature is less quick than the liquefying temperature. This is on the grounds that the Debye temperature fluctuates as square foundation of softening temperature.

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