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Magnetic Properties of Nanostructured Material with the Effect of Dimension

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ABSTRACT

In this Study, Qi model, Jiang model and Lu model, are used to predict the variation of magnetic properties with size and shape in nanosolids. Magnetic properties of nanosolids such as Curie Temperature (Tcn), Magnetization (Msn) and Neel Temperature (T_{nn}) of Cu, Ag are studied. It is predicted that as the size of nanosolids is decreased, all these three properties decrease with decreasing size. These magnetic properties are also studied with different shapes of nanosolids, such as thin films, cylindrical nanowires, spherical, regular tetrahedral nanoparticles and regular triangular cross-section nanowires. The computational results are compared with the available experimental and simulated data to validate our theory.

Keywords: Curie temperature, magnetization, Neel temperature, nanomaterials, shape

I. INTRODUCTION

Unlike bulk material, properties of nanomaterial such as thermodynamic and magnetic properties are affected by the decrease in size and change of shapes in nanomaterials [1-4]. These nanomaterials can be presented in different shapes such as nanorods, thin films, cylindrical nanowires, spherical, rectangular tetrahedral nanoparticles and regular triangular cross-section nanowires. Magnetic and thermodynamic properties of nanomaterials go hand in hand, as we study how they are affected by both decrease in size and the change of shapes of nanomaterials [5-9]. these properties are the Curie temperature, magnetization and Neel temperature.

Curie temperature (T_{cn}) is the temperature above which, certain materials lose their permanent magnetic properties that can be replaced by induced magnetism. Whilst, Magnetization (M_{sn}) is a measure of density of induced magnetic dipole moments in a magnetic material. In addition, Neel temperature (T_{nn}) is the temperature above which an antiferromagnetic substance loses its antiferromagnetism and becomes paramagnetic.

unpaired electrons, as size decreases, the electron spin is disturbed by small temperatures, due to the increase of the surface to volume ratio because of that the atoms in the molecules of nanomaterials pack closer to the surface. The Ferromagnetic nanomaterials display super paramagnetic properties due to the decrease in size and resultant decrease in the Curie temperature. Antiferromagnetic nanomaterials on the other hand, exhibit similar traits as ferromagnetic nanomaterials regardless of the slight difference that due to the electron spin in their atoms, the magnetic moments align in a regular pattern with spins pointing in opposite directions and instead of losing their antiferromagnetic properties at Curie temperature they lose their antiferromagnetic properties at Neel temperature.

For the theoretical procedures, we will look at three models designed by Jiang et al, Lu et al and Qi [10-12]. Jiang et al designed a thermodynamic model to study the size dependence of magnetic properties, thermal properties and mechanical properties of nanomaterials, and this model is called the Jiang model. Lu et al [11] designed a cohesive energy model designed to study the size dependence of saturated magnetization of ferromagnetic nanocrystals at room temperature and this model is the Lu model. Lastly, He at al designed a model to study the effect of size on Curie temperature and magnetization in ferromagnetic nanomaterials and this model is the Qi model [12].

In this contribution, the nanomaterials studied are Cu, Ag and looking at their magnetic properties as they change with the decrease in size of the nanomaterials and putting into consideration different shapes of these nanomaterials.

II. THEORETICAL ANALYSIS

The thermodynamic properties are related to the melting temperature of nanomaterials, according to Qi [12] model, melting temperature is expressed as

$$T_{mn} / T_{mb} = (-3N / 4n) + 1 \tag{1}$$

The melting and Curie temperature are proportional to each other [13], given as

$$T_{mn} / T_{mb} = T_{cn} / T_{cb} \tag{2}$$

To analyze the shape effects, a shape factor γ is added, shape factor is the ratio of the surface areas of non-spherical to spherical shape and the shape factor changes with the change in surface atoms to volume ratio of different shapes. Therefore, from Eq. (1) and (2), the relative Curie temperature of different shapes of nanomaterials are written as

$$T_{cn} / T_{cb} = \gamma(-3N / 4n) + 1 \tag{3}$$

The value of 3N/4n, which depends upon shape of nanosolids is given as 2d/L, d/h, and 3d/D for nanowire, nanofilm and nanosphere respectively [14]. Next parameter, magnetization, which is significant to this study as it tells us at what extent a magnetic material is affected by the outside magnetic field and it causes the spin within the material to align it with the field. According to Rawat and Goyal [15], for ferromagnetic materials, magnetization is given as

$$M_{sn} / \mathrm{M}_{sb} = 4(T_{cn} / T_{cb}) - 3 \tag{4}$$

Also, Neel temperature can be expressed as

$$T_{Nn} / T_{Nb} = \gamma(-3N / 4n) + 1 \tag{5}$$

Jiang model [10] formulates the ratio of Curie temperature in nanomaterial to bulk material as

$$T_{cn} / T_{cb} = \exp(-2\gamma S_b / 3R(D / D_0 - 1)) \tag{6}$$

Here, S_b is the bulk vibrational melting entropy, R is the gas constant and D is the diameter of the nanomaterial and D_0 is the acute size at which all atoms in a nanomaterial are present at the surface. Here, $D_0 = 2h \times (3 - d)$ [16]. In the case of spherical nanomaterials, *d=0* for nanowires *d=1* and for thin film *d=2*.

According to the Jiang model [10], the relative magnetization of nano to bulk material can be obtained by using Eq. (4), which gives

$$M_{sn} / \mathrm{M}_{sb} = 4 \times \exp(-2\gamma S_b / 3R(D / D_0 - 1)) - 3 \tag{7}$$

And Neel temperature is expressed as

$$T_{Nn} / \mathrm{T}_{Nb} = \exp(-2\gamma S_b / 3R(D / D_0 - 1)) \tag{8}$$

According to Lu model [11], relative Curie temperature is written mathematically as

$$T_{cn} / \mathrm{T}_{cb} = \exp(-2\gamma S_b / 3R(D / D_0 - 1)) \times (1 - (1 / (12\,\mathrm{D} / \mathrm{D}_0 - 1))) \tag{9}$$

From Eqs. (4) and (9), The Magnetization can be expressed as

$$M_{sn} / M_{sb} = 4 \times \exp(-2\gamma S_b / 3R(D/D_0 - 1)) \times (1 - (1/12D/D_0 - 1))) \quad (10)$$

And Neel temperature can be written as

$$T_{Nn} / T_{Nb} = \exp(-2\gamma S_b / 3R(D/D_0 - 1)) \times (1 - (1/12D/D_0 - 1))) \quad (11)$$

III. RESULTS AND DISCUSSION

The calculated results for size and shape dependent Curie temperature, magnetization and Neel temperature, using models Eqs. (3) -(11) are reported in figures 1-7. Input parameters required in calculations are given in Tables 1-2. The size dependence of Curie temperature is particularly depicted in figs. 1-4 and the available experimental data is shown as well for comparison purpose. The Curie temperature decreases moderately as the size decreases but when the nanomaterials reach sizes below approximately 15 nm, the decrease in size becomes momentous as seen in figs. 1-4. The same applies for the Neel temperature as seen in fig. 7. Although, for Neel temperature, it decreases significantly much earlier than Curie temperature. The decrease of Neel temperature is moderate until it reaches the sizes approximately below 20nm whereby the decrease of Neel temperature as size decreases becomes momentous.

The most accurate, or rather, precise model being the Qi model aligns closer to the experimental data than Jiang model and Lu model. Figures 2, 4, 5, 6 and 7 show typical examples of trends of different shapes in different nanomaterials.

Table 1 Used parameters [17]

Nanosolids	h **(nm)**	S_b **(J/mol K)**	T_C**(K)**
Cu	0.256	9.76	1357.6
Ag	0.319	9.16	1234

Table 2 Shape factors [15]

Shape of cross section	spherical	tetrahedral	triangular	cylindrical
Shape factor	1	1.49	1.29	1

For copper, figure 1 depicts the size dependence of Curie temperature for spherical nanomaterials as predicted by Qi, Jiang and Lu models [10-12] by using equations (3), (6) and (9) whereby the size varies. As seen, the Qi model [12] is closer to the experimental values [18] given thus the Qi model explains better the size dependence of curie temperature in copper.

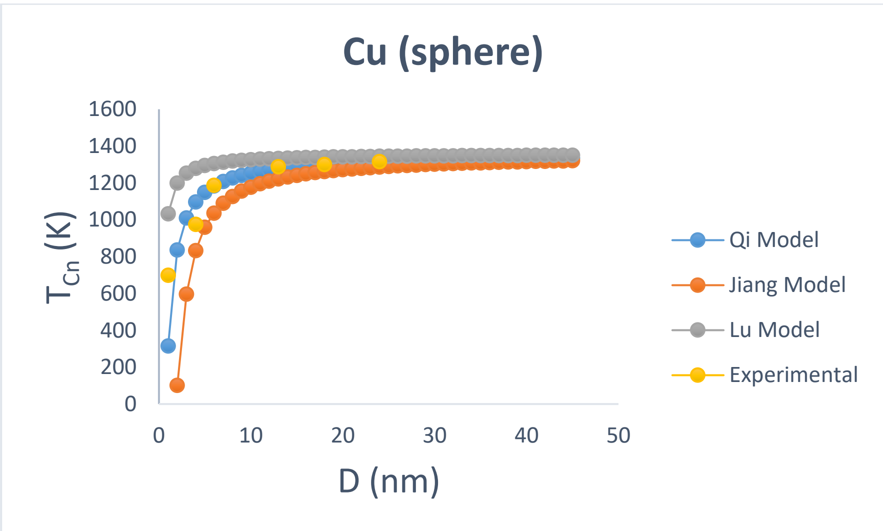

Figure 1: *A graph depicting Curie temperature of Copper (sphere) nanomaterial*

Figure 2 shows the shape and size dependence of Curie temperature in copper. Using equations (3), since the Qi model appears to be the most accurate of the three models proposed. The graph depicts the Curie temperature of spherical nanoparticles, tetrahedral nanoparticles, triangular nanowire, thin film, nanowire and the different trends they show as size of the nanomaterial decreases. It is seen that these trends vary slightly, with the thin film having the highest Curie temperature trend for copper nanomaterials and the tetrahedral nanoparticles having the lowest Curie temperature trend for copper nanomaterials.

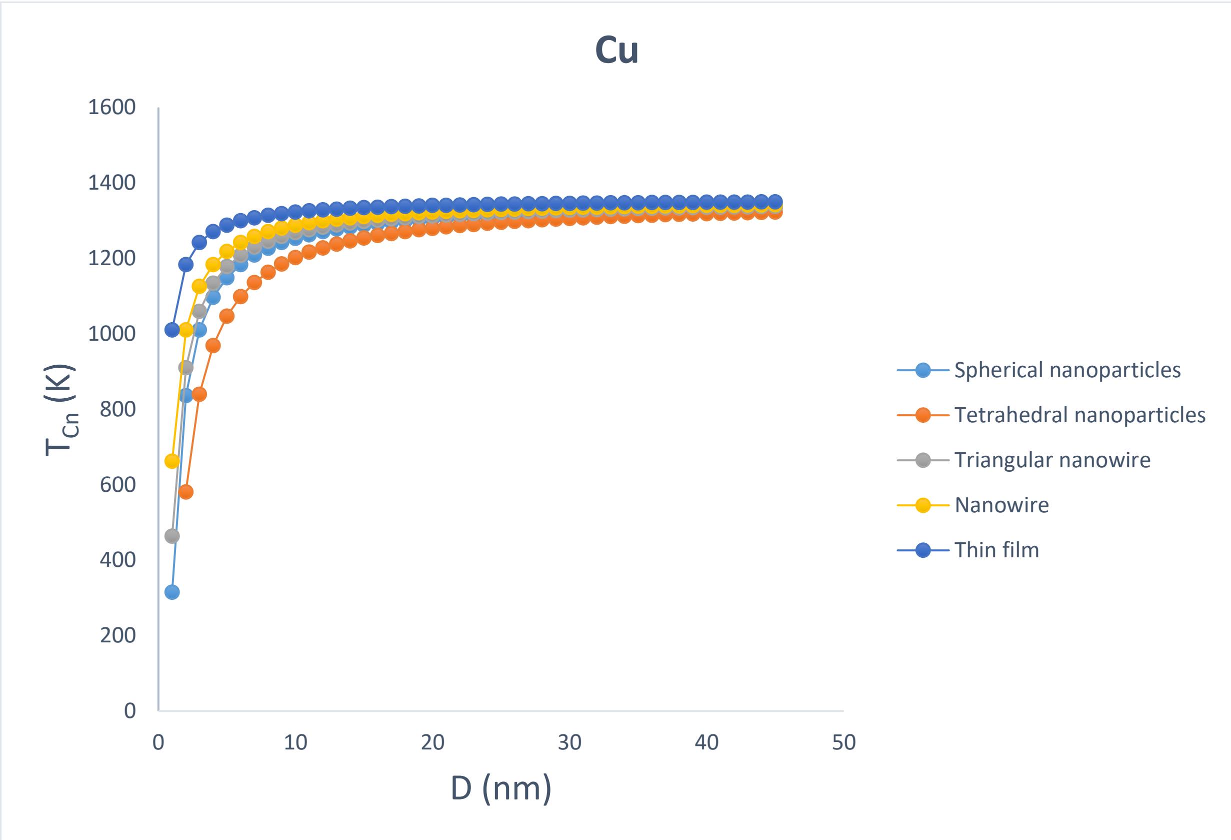

Figure 2: *A graph depicting Curie temperature for different shapes of Copper nanomaterials*

If the Curie temperature is the temperature at which ferromagnetic and ferromagnetic nanomaterials lose their permanent magnetic nature, then for nanomaterials, as the size decreases and atoms are brought closer to the surface, the magnetic moment is easily disturbed at lower temperatures. Thus, the magnetic spins do not align equally in the same direction but rather they become scattered and turning a ferromagnetic nanomaterial into a paramagnetic nanomaterial which needs an external magnetic field to induce magnetism.

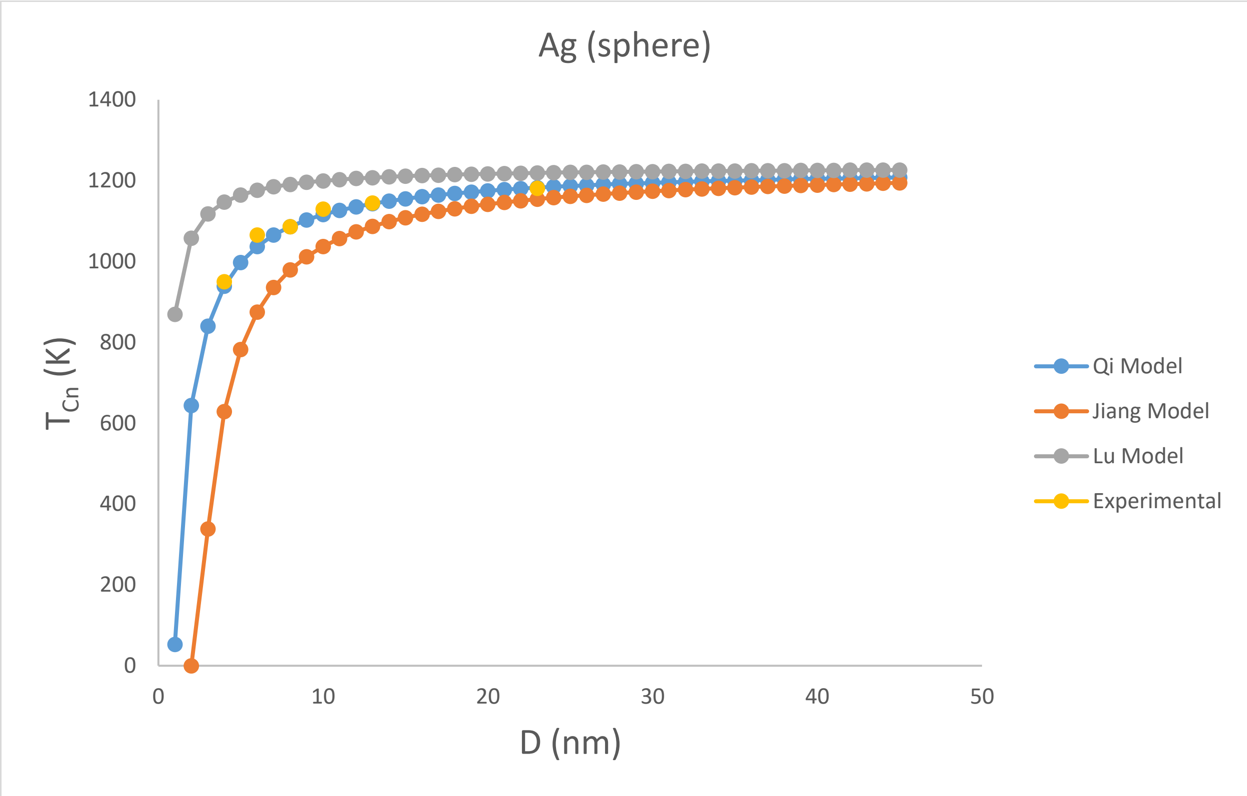

Figure 3: *A graph depicting Curie temperature of Silver (sphere) nanomaterial*

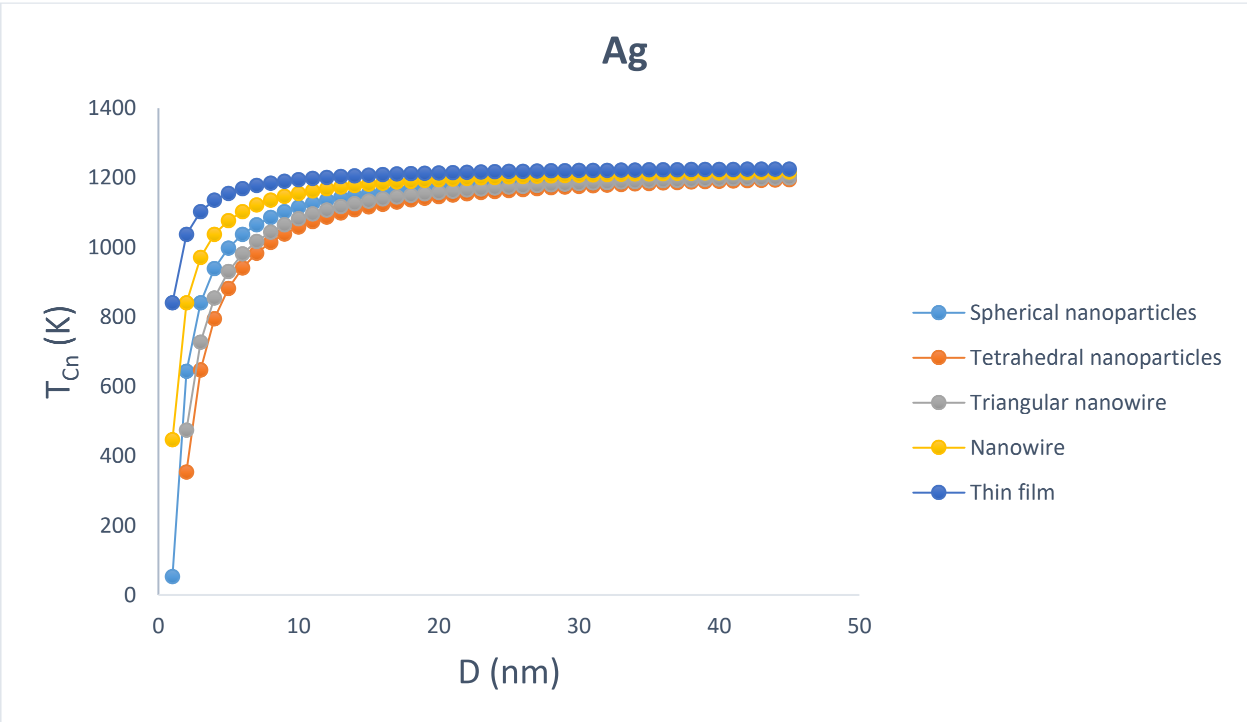

Figure 4: *A graph depicting Curie temperature for different shapes of Silver nanomaterials*

Magnetisation, as seen in Eqs. (4), (7) and (10), can be derived from Curie temperature. Similar to Curie temperature, the size and shape dependence of magnetization is studied by using the Qi model, Jiang model and Lu model [10-12]. For this study, nanomaterials used are Copper (Cu), Silver (Ag). Similar to Curie temperature, magnetization is described through magnetic dipole moments. As the size of nanomaterials decreases and the surface to volume ratio increases, magnetization decrease. This is seen in figs. 5-6 below, which depict the trend of magnetization as predicted though Qi model, Jiang model and Lu model. The decrease in magnetization is much greater than of Curie temperature but the drop seems to be uniform than in Curie temperature.

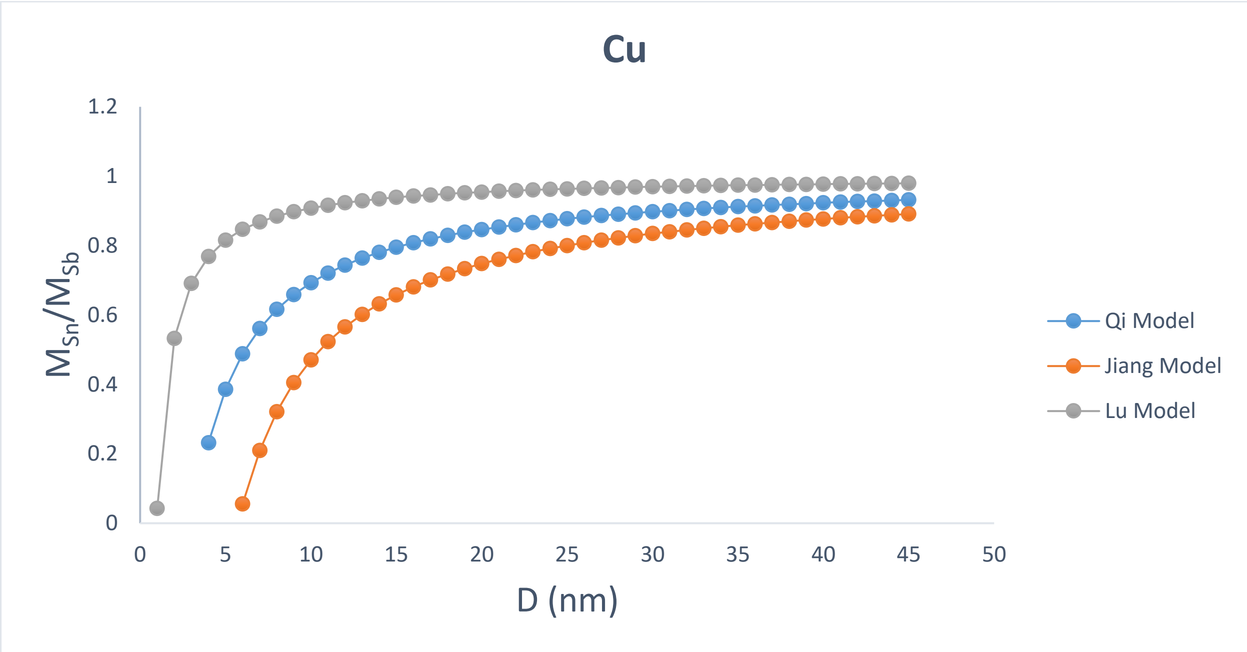

Figure 5: *A graph depicting relative magnetization of Copper (sphere) nanomaterial*

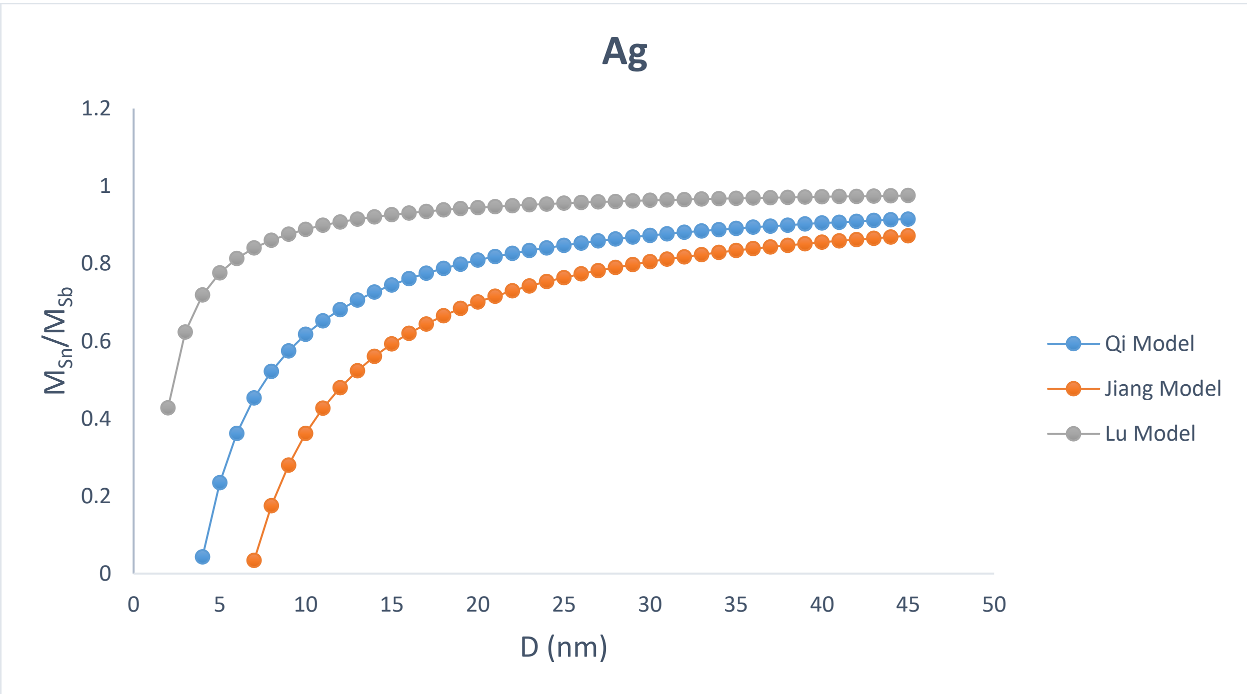

Figure 6: *A graph depicting relative magnetization of Silver (sphere) nanomaterial*

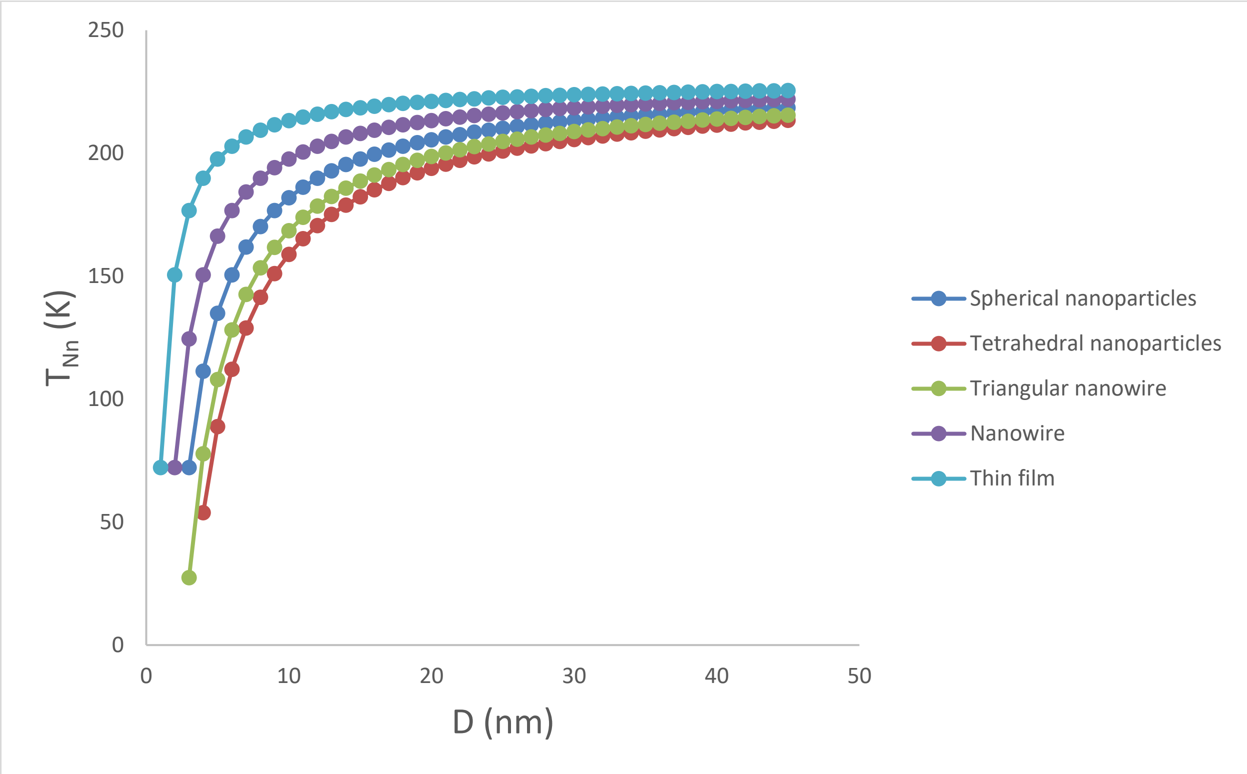

Figure 7: *A graph depicting Neel Temperature of Copper (sphere) nanomaterial*

Neel temperature on the other hand, unlike Curie temperature, is the temperature at which antiferromagnetic materials become paramagnetic. That is, magnetic spins, which were aligned in different directions, now become scattered in the absence of a magnetic field.

Fig. 7 show the size and shape dependence of Neel temperature in Cu nanomaterial in the form of different shapes that are spherical nanoparticles, tetrahedral nanoparticles, triangular nanowire, nanowire and thin film. As seen, the drop in the Neel temperature with size reduction is the least in thin films and is maximum in tetrahedral nanoparticles. For antiferromagnetic nanomaterials, Neel temperature shows their phase stability. Similar to magnetization and Curie temperature, Neel temperature is stronger for fcc and hcp than bcc because of the tightly packed atoms within an antiferromagnetic nanocrystal. These three properties, Curie temperature, magnetization and Neel temperature are all size and shape dependent in nanomaterials.

IV. CONCLUSION

In this paper, we have studied the size and shape dependence of magnetic properties in nanosolids by modelling using Qi model, Jiang model and Lu model. These three magnetic properties, which are namely Curie temperature, magnetization and Neel temperature were found to decrease as size of the nanomaterials decreases. These properties share this same effect from size and shape because of the increase in surface to volume ratio. From studying these three properties and their size and shape dependence, the Qi model is seen to be the most accurate of the three models or rather it is closest to the experimental data.

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