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Modelling to determine the variation of magnetic properties with size and shape in the nanomaterials

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Abstract. Three different models, viz. Qi model, Jiang model and Lu model, have been used in the present paper for studying the size and shape dependence of magnetic properties of the nanomaterials. The magnetic properties considered here are Curie temperature (T_{C}), magnetisation (M_{S}) and Neel temperature (T_{N}). It is observed that Curie temperature, magnetisation and Neel temperature decrease with decrease in the size of the nanomaterial. This decrease is due to the increase in the surface atoms with reduction in size. The variations in Curie temperature, magnetisation and Neel temperature are studied for cylindrical nanowires, thin films, spherical, regular tetrahedral nanoparticles, and regular triangular cross-section nanowires. The models used in the study give similar trend of variation and after the comparison of the computed results with experimental data, it is found that Qi model works well compared to Lu and Jiang models. A close agreement between the available experimental results and the calculated results from Qi model justifies the validity of the present work.

Keywords. Curie temperature; magnetisation; Neel temperature; size; shape.

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1. Introduction

The emerging field of nanoscience and nanotechnology is attracting the attention of the researchers world-wide and it is presently a multidisciplinary and broadest research field. Physics of nanomaterials is very important and it is different from their counterpart bulk materials because of their unique properties. Nanomaterials possess fascinating chemical, physical, mechanical, thermodynamical and magnetic properties, compared to the macroscopic particles due to their large surface to volume ratio [1–5]. Fabrication of magnetic nanomaterials may help to study their properties by using experimental techniques. There is a great impact of size, shape and dimensionality on the properties of nanomaterials because of the presence of a large number of surface atoms in the nanomaterials [6–8]. In the era of nanotechnology, magnetic systems of low dimensions like nanorods, thin films, multilayers and nanoparticles have attracted the attention of researchers for applications in all fields of science [9–12]. By reducing the size of the magnetic material to the nanolevel, magnetic solids may depict different behaviours. It is obvious from the previous studies that the Curie temperature of ferromagnetic nanomaterials decreases as their size is reduced to nanoscale and this targets new methods of fabrication of new functional nanomaterials having a wide variety of applications. Properties of ferroelectric materials are influenced by the decrease in size and this is a subject of theoretical importance as well as practical importance [13–17].

There are magnetic nanoparticles having unique physical, chemical and magnetic properties and have applications in vast areas of high-density perpendicular recordings, ultrahigh frequency devices, colour imaging and magnetic refrigeration [18–20]. Many experimental studies have been done by scientists to fabricate nanomaterials and to explore their properties. Also, theoretical studies and molecular dynamic simulations have been carried out to predict the properties of magnetic nanomaterials. Jiang *et al* [17] studied the size dependence of magnetic properties, thermal properties and mechanical properties by using a thermodynamic model. Lu *et al* [21] studied the size-dependent saturated magnetisation of ferromagnetic nanocrystals at room temperature with the help of cohesive energy model. He *et al* [13] investigated experimentally and theoretically the effect of size on magnetic properties of Ni nanoparticles and observed that Curie temperature and magnetisation tend to decrease with reduction in the size of nanoparticles.

In the present paper, the authors have studied the effect of size, shape and dimensionality on magnetic properties, viz. Curie temperature (T_C), magnetisation (M_S) and Neel temperature (T_N) of the nanomaterials. Three simple size- and shape-dependent models, Qi model [22], Jiang model [23] and Lu model [24], are considered here to know the impact of size and shape on the magnetic properties in nanomaterials. The nanomaterials taken here to study the variation of these magnetic properties with size are Ni, Fe_3O_4, Co and CuO taking cylindrical nanowires, thin films and spherical nanoparticles into consideration. The results from these three models are then compared with the previous available data to find the best model to study magnetic properties of nanomaterials.

2. Methodology

According to Qi model [22], the relative melting temperature in the nanomaterials to bulk is given by

$$\frac{T_{\mathrm{Mn}}}{T_{\mathrm{Mb}}} = 1 - \frac{3N}{4n}, \tag{1}$$

where T_{Mn}, T_{Mb} are melting temperatures of nano and bulk material, N is the number of atoms on the surface of the nanomaterial and n is the total number of atoms.

For ferromagnetic and antiferromagnetic nanocrystals, which have the same structure as the bulk materials, the Curie temperature T_C and Debye temperature θ_D are related as [12,25]

$$\frac{T_{\mathrm{Cn}}}{T_{\mathrm{Cb}}} = \frac{\theta_{\mathrm{Dn}}{}^2}{\theta_{\mathrm{Db}}^2}. \tag{2}$$

Here T_{Cn}, θ_{Dn} are the Curie temperature and the Debye temperature of the nanomaterial and T_{Cb} and θ_{Db} represent the Curie temperature and the Debye temperature of the bulk nanomaterial respectively.

Relation between the melting temperature and theDebye temperature is given by Liang and Baowen as follows [26]:

$$\frac{T_{\mathrm{Mn}}}{T_{\mathrm{Mb}}} = \frac{\theta_{\mathrm{Dn}}{}^2}{\theta_{\mathrm{Db}}^2}. \tag{3}$$

Combining eqs (2) and (3), the relation obtained between Curie temperature and melting temperature is as follows:

$$\frac{T_{\mathrm{Mn}}}{T_{\mathrm{Mb}}} = \frac{T_{\mathrm{Cn}}}{T_{\mathrm{Cb}}} = 1 - \frac{3N}{4n}. \tag{4}$$

Shape factor λ is inserted in eq. (4) to analyse the shape effect of the nanomaterials, and the relative Curie temperature in nanomaterial to bulk is expressed as

$$\frac{T_{\mathrm{Cn}}}{T_{\mathrm{Cb}}} = 1 - \lambda\frac{3N}{4n}, \tag{5}$$

where λ is the shape factor and it is the ratio of the surface areas of non-spherical to spherical shape. It can also be defined as the ratio of surface area of the non-cylindrical nanowires to the surface area of the cylindrical nanowires. The value of λ varies with change in surface atoms to volume ratio for different shapes.

Here $\frac{N}{2n}$ depends on the shape of the nanomaterial and its value for the nanowire, thin film and sphere shape are deduced as $\frac{4d}{3L}$, $\frac{2d}{3h}$ and $\frac{2d}{D}$ respectively [7].

For the nanowire, thin film and spherical shape of the nanomaterial, the relative Curie temperature in the nanomaterial to bulk can be expressed as follows:

$$\frac{T_{\mathrm{Cn}}}{T_{\mathrm{Cb}}} = 1 - \lambda\frac{2d}{L} \tag{5a}$$

$$\frac{T_{\mathrm{Cn}}}{T_{\mathrm{Cb}}} = 1 - \lambda\frac{d}{h} \tag{5b}$$

$$\frac{T_{\mathrm{Cn}}}{T_{\mathrm{Cb}}} = 1 - \lambda\frac{3d}{D}. \tag{5c}$$

Magnetisation is a very important property of a magnetic material which tells us to what extent it is affected by the external magnetic field and it causes the spins within a material to align with the field. Saturation magnetisation is the maximum value of magnetisation in this state. For ferromagnetic materials, the relation between Curie temperature and magnetisation is as follows [12]:

$$\frac{M_{\mathrm{Sn}}}{M_{\mathrm{Sb}}} = 4\left[\frac{T_{\mathrm{Cn}}}{T_{\mathrm{Cb}}}\right] - 3, \tag{6}$$

where M_{Sn}, M_{Sb} are the saturated magnetisation of the nano and bulk materials.

Equation (6) shows that the repression in magnetisation is around four times the Curie temperature and it is due to the increase in surface atoms.

By inserting the value of $\frac{T_{\mathrm{Cn}}}{T_{\mathrm{Cb}}}$ from eq. (5) into eq. (6), the final expression for the magnetisation obtained using Qi model is as follows:

$$\frac{M_{\mathrm{Sn}}}{M_{\mathrm{Sb}}} = 4\left(1 - \lambda\frac{3N}{4n}\right) - 3. \tag{7}$$

For the nanowire, thin film and sphere shapes, the final expressions for magnetisation can be written by substituting the value of $\frac{N}{2n}$ in eq. (7).

Neel temperature is a very important physical quantity which describes the phase stability of antiferromagnetic nanocrystals. According to the magnetic field theory [12], Neel temperature ratio in nano to bulk is found to be similar to the ratio of Curie temperature in nano to bulk and can be expressed as

$$\frac{T_{\mathrm{Nn}}}{T_{\mathrm{Nb}}}=\frac{T_{\mathrm{Cn}}}{T_{\mathrm{Cb}}}. \tag{8}$$

In view of eq. (5), relative Neel temperature in nano to bulk can be expressed as follows:

$$\frac{T_{\mathrm{Nn}}}{T_{\mathrm{Nb}}}=1-\lambda\frac{3N}{4n}. \tag{9}$$

Equations (5), (7) and (9) are the required expressions to find the variation of Curie temperature, magnetisation and Neel temperature in the magnetic nanomaterials using Qi model.

According to Jiang model [23,27], the expression for the ratio of melting temperature of nanomaterial to bulk is as follows:

$$\frac{T_{\mathrm{Mn}}}{\mathrm{T}_{\mathrm{Mb}}}=\exp\left[\frac{-2\lambda S_{\mathrm{b}}}{3R\left(\frac{D}{D_0}-1\right)}\right], \tag{10}$$

where S_{b} is the bulk vibrational melting entropy, R is a constant, λ is the shape factor, D is the diameter of the nanomaterial.

Here D_0 is given by [2]

$$D_0=2(3-d)*h, \tag{11}$$

where d is the degree of freedom and h is the atomic diameter. For spherical nanoparticles $d = 0$ and for nanowires and thin films, it is 1 and 2 respectively. D_0 is the critical size when all the atoms are present on the surface of the nanomaterial.

In the view of eq. (4), the Curie temperature relation can be expressed as follows:

$$\frac{T_{\mathrm{Cn}}}{T_{\mathrm{Cb}}}=\exp\left[\frac{-2S_{\mathrm{b}}}{3R\left(\frac{D}{D_0}-1\right)}\right]. \tag{12}$$

In the case of nanowires, thin film and spherical nanomaterial, the expression for Curie temperature can be obtained using eq. (11) in eq. (12) as follows:

$$\frac{T_{\mathrm{Cn}}}{T_{\mathrm{Cb}}}=\exp\left[\frac{-2S_{\mathrm{b}}}{3R\left(\frac{D}{4h}-1\right)}\right] \tag{12a}$$

$$\frac{T_{\mathrm{Cn}}}{T_{\mathrm{Cb}}}=\exp\left[\frac{-2S_{\mathrm{b}}}{3R\left(\frac{D}{2h}-1\right)}\right] \tag{12b}$$

$$\frac{T_{\mathrm{Cn}}}{T_{\mathrm{Cb}}}=\exp\left[\frac{-2S_{\mathrm{b}}}{3R\left(\frac{D}{6h}-1\right)}\right]. \tag{12c}$$

Table 1. Input parameters required in the present work [12,21,25,28–30].

Nanomaterial	h (nm)	S_{b} (J/mol K)	T_{C} (K)	T_{N} (K)
Ni	0.2492	10.12	630	
$\mathrm{Fe_3O_4}$	0.222	10.55	860	
Co	0.2497	9.157	1404	
CuO	0.6845	7.016		229
NiO	0.842	7.271		523

Table 2. Values of shape factors for different shapes [27,31].

Shape	Shape factor
Sphere nanoparticles	1
Regular tetrahedral nanoparticles	1.49
Cylindrical nanowire	1
Regular triangular nanowires	1.286

In view of Jiang model, ratio of magnetisation in the ferromagnetic nano to bulk material can be obtained using eq. (6) as follows:

$$\frac{M_{\mathrm{Sn}}}{M_{\mathrm{Sb}}}=4*\exp\left[\frac{-2S_{\mathrm{b}}}{3R\left(\frac{D}{D_0}-1\right)}\right]-3. \tag{13}$$

The expression for Neel temperature with the help of Jiang model can be written using eq. (8) as

$$\frac{T_{\mathrm{Nn}}}{T_{\mathrm{Nb}}}=\exp\left[\frac{-2S_{\mathrm{b}}}{3R\left(\frac{D}{D_0}-1\right)}\right]. \tag{14}$$

Expression of magnetisation and Neel temperature for nanowires, thin films and spherical nanomaterial can be obtained by substituting D_0 in eqs (13) and (14) respectively.

Equations (12)–(14) are the expressions used to predict the variation of Curie temperature, magnetisation and Neel temperature due to the effect of size, shape and dimension on the nanomaterials using Jiang model.

In accordance with Lu model [24], the expression for the melting temperature can be written as follows:

$$\frac{T_{\mathrm{Mn}}}{T_{\mathrm{Mb}}}=\left[1-\frac{1}{\frac{12D}{D_0}-1}\right]\exp\left[\frac{-2\lambda S_{\mathrm{b}}}{3R\left(\frac{12D}{D_0}-1\right)}\right]. \tag{15}$$

From eqs (4) and (15), the expression for the Curie temperature can be written as

$$\frac{T_{\mathrm{Cn}}}{T_{\mathrm{Cb}}}=\left[1-\frac{1}{\frac{12D}{D_0}-1}\right]\exp\left[\frac{-2\lambda S_{\mathrm{b}}}{3R\left(\frac{12D}{D_0}-1\right)}\right]. \tag{16}$$

The symbols in eq. (16) are the same as the symbols explained in Jiang model.

Considering the case of nanowires, thin films and spherical nanomaterials, Curie temperature can be expressed as follows:

$$\frac{T_{\mathrm{Cn}}}{T_{\mathrm{Cb}}} = \left[1 - \frac{1}{\frac{12D}{4h} - 1}\right] \exp\left[\frac{-2\lambda S_{\mathrm{b}}}{3R\left(\frac{12D}{4h} - 1\right)}\right] \tag{16a}$$

$$\frac{T_{\mathrm{Cn}}}{T_{\mathrm{Cb}}} = \left[1 - \frac{1}{\frac{12D}{2h} - 1}\right] \exp\left[\frac{-2\lambda S_{\mathrm{b}}}{3R\left(\frac{12D}{2h} - 1\right)}\right] \tag{16b}$$

$$\frac{T_{\mathrm{Cn}}}{T_{\mathrm{Cb}}} = \left[1 - \frac{1}{\frac{12D}{6h} - 1}\right] \exp\left[\frac{-2\lambda S_{\mathrm{b}}}{3R\left(\frac{12D}{6h} - 1\right)}\right]. \tag{16c}$$

The expression for magnetisation and Neel temperature of the nanomateials with the help of Lu model can be written using eqs (6) and (8) as follows:

$$\frac{M_{\mathrm{Sn}}}{M_{\mathrm{Sb}}} = 4\left[1 - \frac{1}{\frac{12D}{D_0} - 1}\right] \exp\left[\frac{-2\lambda S_{\mathrm{b}}}{3R\left(\frac{12D}{D_0} - 1\right)}\right] - 3 \tag{17}$$

$$\frac{T_{\mathrm{Nn}}}{T_{\mathrm{Nb}}} = \left[1 - \frac{1}{\frac{12D}{D_0} - 1}\right] \exp\left[\frac{-2\lambda S_{\mathrm{b}}}{3R\left(\frac{12D}{D_0} - 1\right)}\right]. \tag{18}$$

Equations (16)–(18) are the expressions used to predict the Curie temperature, magnetisation and Neel temperature in magnetic nanomaterials with the help of a quantitative Lu model [24].

3. Results and discussion

From the above discussion, it is very obvious that three qualitative models, viz. Qi model, Jiang model and Lu model, are used for the comparative study of size, shape and dimensionality dependence of magnetic properties of the nanomaterials. The input parameters required in the calculations of magnetic properties, i.e. Curie temperature, magnetisation and Neel temperature with size and shape are listed in table 1 and values of the shape factors for different shapes are given in table 2. The variation of Curie temperature with size is calculated with the help of eqs (5), (12) and (16) of the Qi model [22], Jiang model [23] and Lu model [24] respectively. The variation of magnetisation with size is calculated with the help of eqs (7), (13) and (17) and the variation of Neel temperature with size is calculated with the help of eqs (9), (14) and (18) using the considered three models respectively.

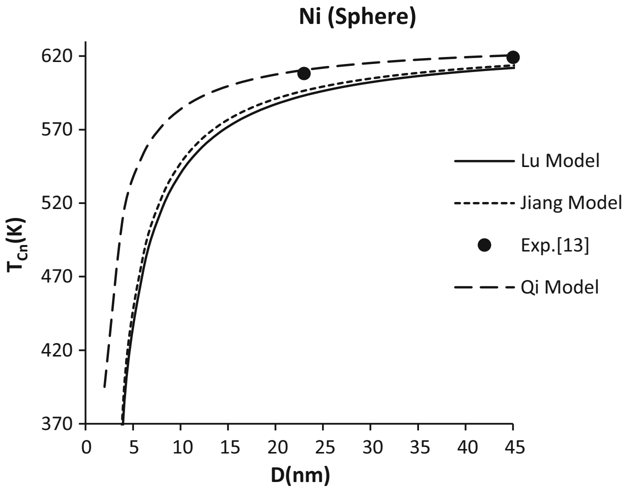

Figure 1. Curie temperature vs. diameter in Ni (sphere) nanomaterial.

Curie temperature, magnetisation and Neel temperature vary with D which is the diameter or the height of the nanostructure. The variation of Curie temperature with size of the spherical Ni nanomaterial using the three models and experimental data [13] is shown in figure 1. Results obtained from the three models show similar trend of variation and the experimental data are observed to be closer to the predicted results obtained from the Qi model. However, it can be seen that the predicted values using Lu and Jiang models deviate from the experimental results. In the case of $\mathrm{Fe_3O_4}$ nanoparticles, the Curie temperatures calculated using the three models and the available experimental data are shown in figure 2. From figure 2, it is observed that the experimental data lie between the Qi and Jiang model results. However, experimental data are closer to the Qi model results and so it is seen that Qi model explains well the variation in Curie temperature with the size of the $\mathrm{Fe_3O_4}$ nanoparticle. Variation of Curie temperature with size for Ni nanostructures of different shapes, viz., cylindrical nanowires, thin film, spherical and regular tetrahedral nanoparticles and regular triangular nanowire is shown in figure 3. For the shapes considered here, the variation of Curie temperature with size of the cobalt nanomaterial is shown in figure 4. From figures 1–4, it is observed that the Curie temperature decreases with decrease in size of the nanomaterial. It is clear from figures 3 and 4 that the Curie temperature falls sharply for small sized nanomaterial, approx. below 10 nm, and this sharp fall in T_{Cn} of the nanomaterials is due to the presence of large number of atoms on the surface of the nanomaterials compared to atoms in volume with decrease in size. For a particular size, Curie temperature is maximum for nanofilms

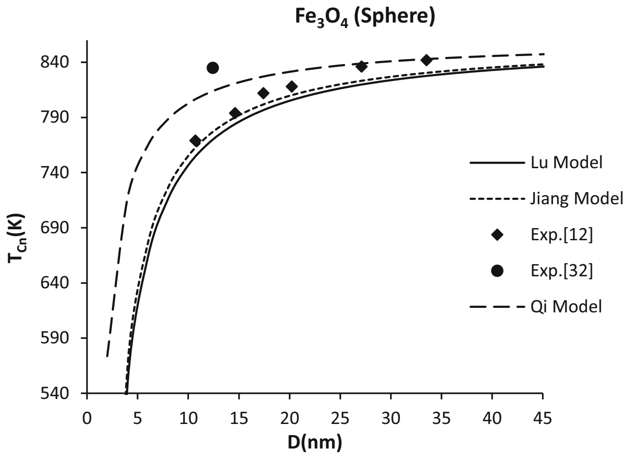

Figure 2. Curie temperature vs. diameter in Fe_3O_4 (sphere) nanomaterial.

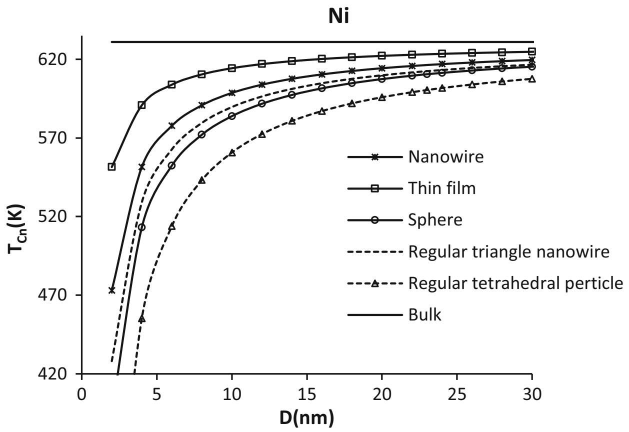

Figure 3. Variation of Curie temperature with diameter for Ni nanomaterial of different shapes.

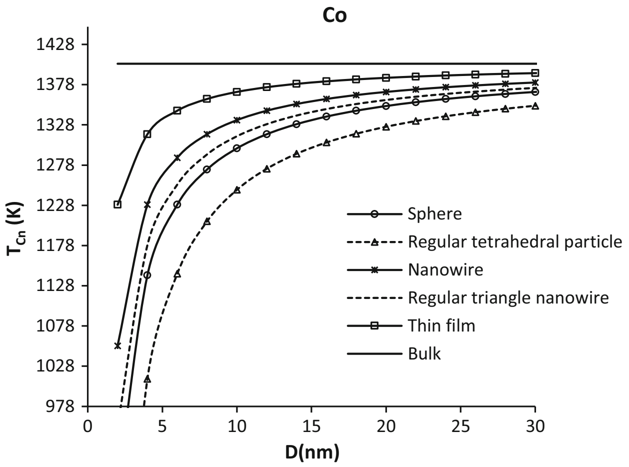

Figure 4. Variation of Curie temperature with diameter for the Co nanomaterial of different shapes.

and minimum for regular tetrahedral shape. In nanomaterials, the effect of shape is found more prominent for smaller size due to the increase in surface to volume ratio but as the size approaches the size of the bulk, the effect of shape decreases.

Now, the theory of Curie temperature is extended to study some other properties of the nanomaterials. The formulation of Curie temperature is extended to get final expression for magnetisation. The variations of magnetisation with size are studied using the Qi, Jiang and Lu models for Ni, Fe_3O_4 and Co nanomaterials and the predicted results are shown in figures 5–8. The available experimental results are also inserted in the respective figures for comparison to judge the best suited model. From the figures, it is observed that the results of all the models show similar trend of variation and a decrement in the magnetisation is observed as the size of the nanomaterial is reduced. The suppression in magnetisation is more than that of the Curie temperature because of the drop in the exchange interaction energy. It is due to the increase in surface atoms which results in the weakening of interspin interaction and thus the magnetisation is reduced with reduction in size at the nanolevel. It is found from the figures that the results of the Qi model are in good agreement with the experimental values of the previous workers for the considered nanomaterials. Variations of magnetisation with size for Ni and Co nanomaterials of different shapes, viz., nanowire, thin film, spherical and regular tetrahedral particles and regular triangular nanowire are shown in figures 7 and 8 respectively.

Saturation magnetisation and Curie temperature are related. The formulation of saturation magnetisation is obtained by extending eq. (8) which indicates that reduction in magnetisation in the nanomaterials is about four times that of the Curie temperature. Both Curie temperature and saturation magnetisation of nanoparticles is also affected by the crystal structure because all have different Curie temperatures due to magnetic moments reacting to their neighbouring electron spins. As fcc and hcp are closed packed structures unlike bcc, their Curie temperatures are higher than bcc as the magnetic moments have stronger effects when molecules are closer. It can be explained in view of the drop in atomic cohesive energy in nanomaterials due to the increase of surface atoms, leading to the weakening of interspin interaction and thus the suppression of magnetisation with reduction in size [21,32,33]. Magnetisation also depends on shape. With change in the surface atoms, magnetisation is found to increase from tetrahedral shape to nanofilm for all the nanomaterials considered in the present paper [8,9,34].

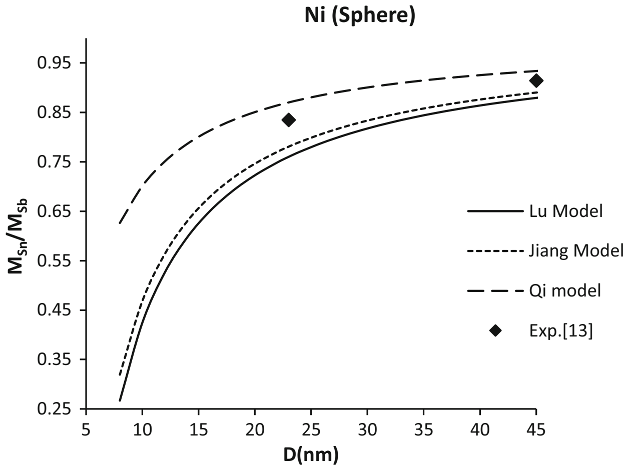

Figure 5. Relative magnetisation vs. diameter in Ni (sphere) nanomaterial.

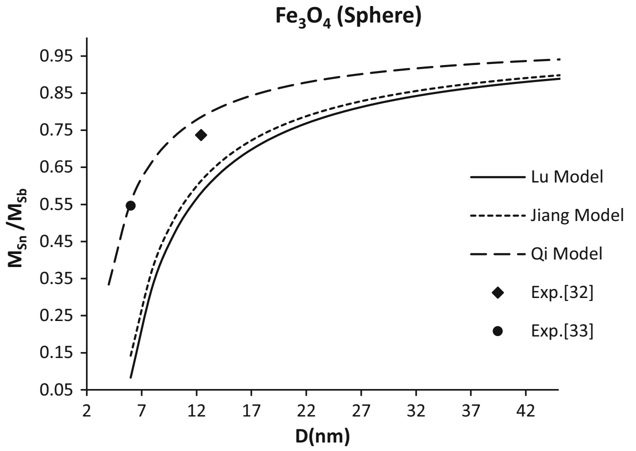

Figure 6. Relative magnetisation vs. diameter in Fe_3O_4 (sphere) nanomaterial.

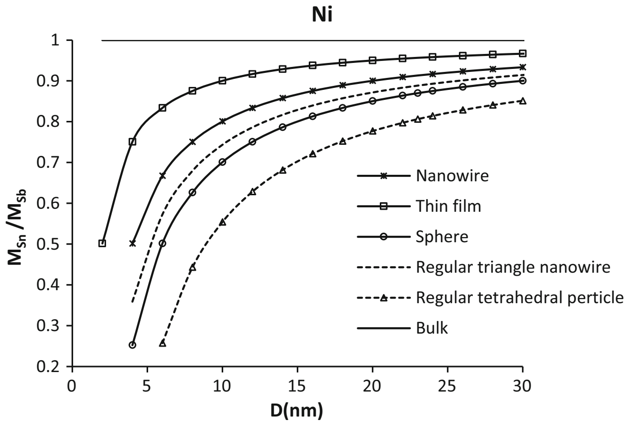

Figure 7. Variation of magnetisation with diameter for Ni nanomaterial of different shapes.

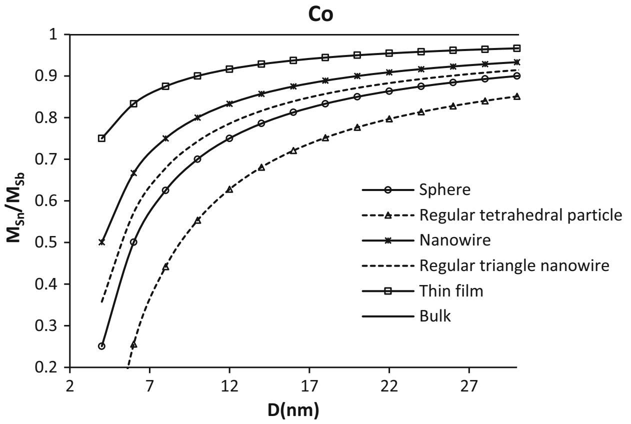

Figure 8. Variation of relative magnetisation with diameter in Co nanomaterial of different shapes.

Neel temperature is another important property of the antiferromagnetic nanomaterials. It is discussed that relative variation in Neel temperature (T_N) is the same as in Curie temperature (T_C). Figure 9 shows the variation of Neel temperature with size using the Qi, Jiang and Lu models for CuO nanomaterials. The available experimental data are also shown in the figure for comparison to judge the best model. Results computed for Neel temperature variation with respect to size with the help of Qi model are in close agreement with the experimental data. Variation of Neel temperature with size for NiO nanomaterial with the help of Qi model along with experimental results is shown in figure 10. These nanomaterials are selected as experimental data because comparison is available for them and is depicted in the respective figures. From figures 9 and 10, it is observed that Neel temperature is decreased with the reduction in size of the nanomaterial and there is a sharp fall in Neel temperature for diameters below 15 nm. The size dependence of antiferromagnetic materials can be explained on the basis of imbalance of the number of up- and down-spins with decrease in size of the material leading to enormous number of surface atoms in the nanomaterials. It is clear from the figures that Qi model works well for the considered nanomaterials compared to Jiang and Lu models. Variations of Neel temperature with size in CuO nanomaterial of different dimensions and shapes are shown in figure 11. It is found that drop in the Neel temperature with size reduction is the least in thin films and is maximum in regular tetrahedral nanoparticles.

Neel temperature is an important physical quantity of antiferromagnetic materials which indicate their phase stability. For free-standing antiferromagnetic nanocrystals, Neel temperature continuously decreases with decrease in size due to the increase of surface/volume ratio. It is found from experimental studies on CuO [35] that with reduction in particle size in CuO nanoparticles

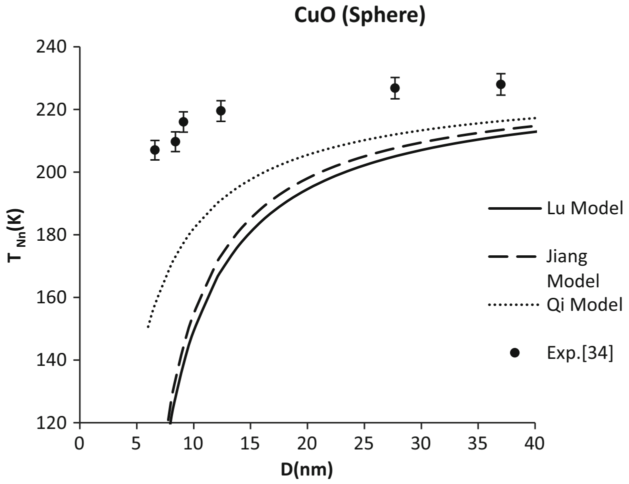

Figure 9. Neel temperature vs. diameter in CuO (sphere) nanomaterial.

from 37 to 10 nm, unit cell volume increases and Neel temperature decreases. The changes in Neel temperature and the lattice constant with particle size may be interpreted in terms of the magnetic Gruneisen parameter. The decrease is most likely triggered by the weaker interchain exchange interaction [35]. With decrease in size of the material, a net magnetic moment is produced due to the non-exact compensation of the two magnetic sublattices, i.e., imbalance in the number of up- and down-spins resulting in the decrease in Neel temperature [32].

The shape, size and the crystal morphology also affect the Neel temperature of the magnetic nanomaterials. This is because of the change in surface atoms with the change in shape and packing fraction of the crystal. Depression of Neel temperature in magnetic nanocrystals is somewhat similar to the melting of free-standing nanoparticles [21,32].

In figures 12 and 13, the percentage deviation between the calculated and experimental data available for Curie temperature and magnetisation of Ni spherical nanoparticles with size is depicted for the models considered in the study. In figure 14, the percentage deviation of the Neel temperature with size in CuO (sphere) nanomaterial is depicted. From the figures, it is observed that the percentage deviation between the calculated and the available experimental values is least from Qi model. A good agreement of the predicted results of the magnetic properties from the Qi model with the experimental data of the previous workers demonstrate the superiority of the Qi model over Jiang and Lu models for all the considered nanomaterials. The present study may help the researchers involved in the fabrication of the nanomaterials by providing them insight about the variation of magnetic properties of the nanomaterials.

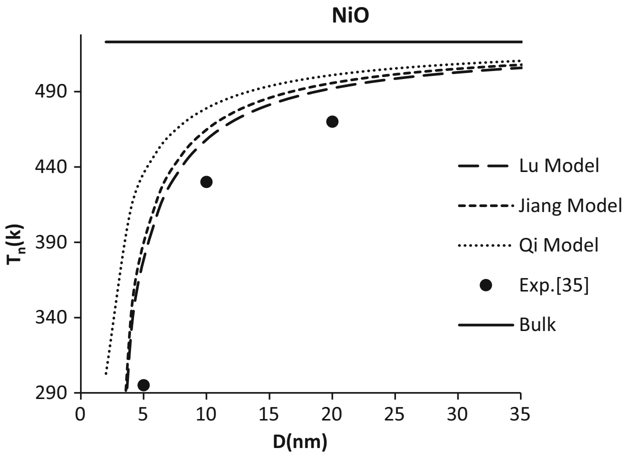

Figure 10. Neel temperature vs. diameter in NiO thin films.

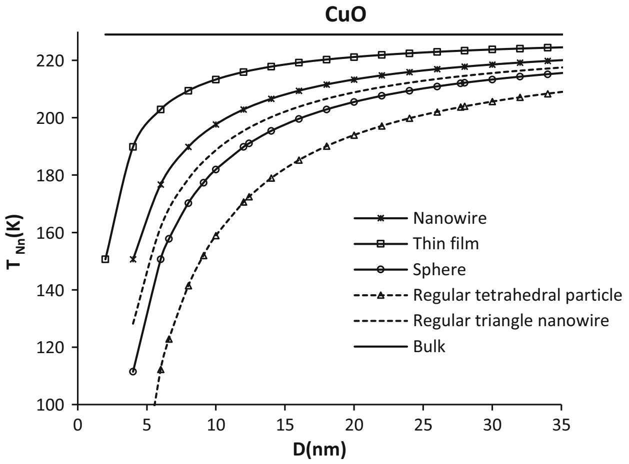

Figure 11. Neel temperature vs. diameter for CuO nanomaterial of different shapes.

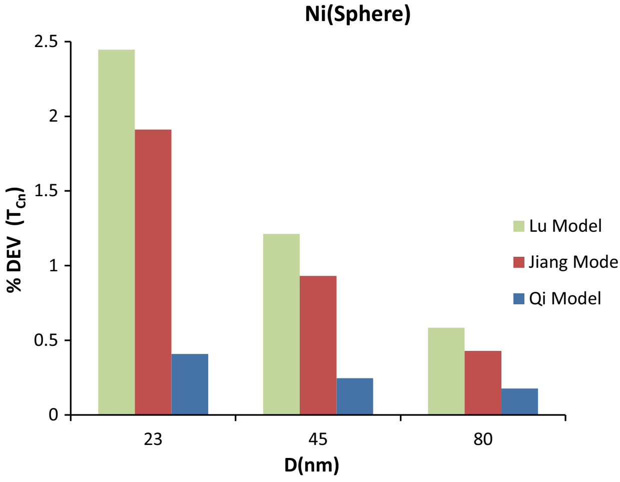

Figure 12. Percentage deviation of Curie temperature with diameter for Ni nanomaterial.

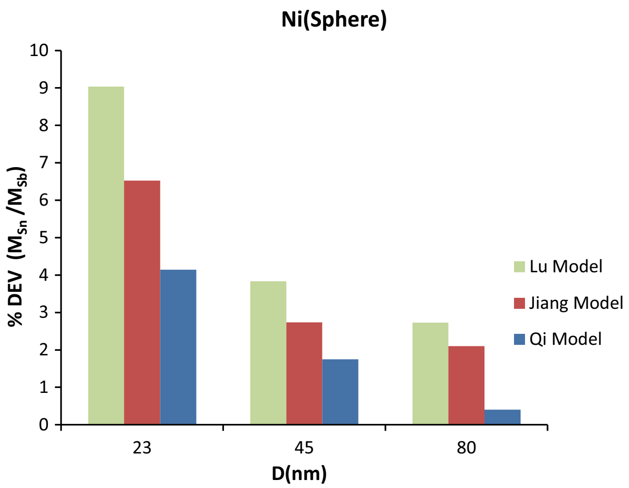

Figure 13. Percentage deviation of magnetisation with diameter for Ni (sphere) nanomaterial.

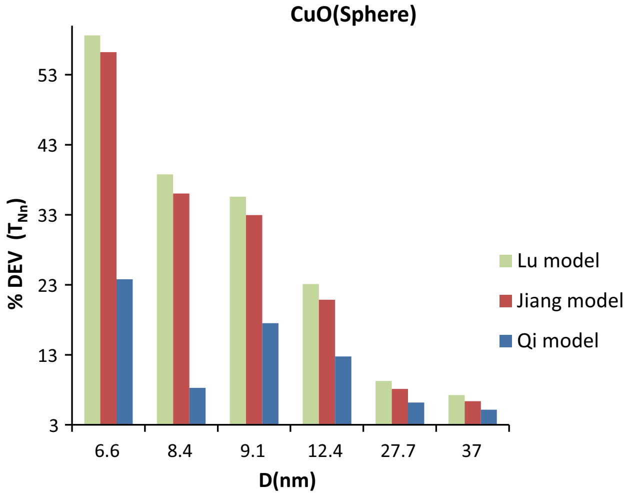

Figure 14. Percentage deviation in Neel temperature with diameter for CuO (sphere) nanomaterial.

The nanomaterials considered in the present study are Ni, Co, Fe_3O_4, NiO and CuO. These materials show distinct magnetic properties as the magnetic properties of the nanomaterials can be material-specific. The magnetic properties may be influenced by the method of synthesis and also by the method of sample preparation for magnetic measurements. In addition, the magnetic behaviour of nanoparticles is also controlled by factors such as their size, composition, shape, crystalline structure and presence of lattice defects [37–39].

The present results for Ni spherical nanoparticles are compared with the experimental results obtained by He *et al* [13]. In [13], Ni nanoparticles were synthesised at different temperatures and have face centred cubic structure. Experimental data for Fe_3O_4 nanoparticle of 12.4 nm size are taken from ref. [36] according to which Fe_3O_4 crystallises in cubic structure. The reduction of the saturation magnetisation in Fe_3O_4 nanoparticle may be attributed to the presence of non-magnetic layer at the particle surface, superparamagnetic relaxation and spin canting [36]. Previous study [37] reveals that in Co nanoparticles, the structural transformation from the bulk hexagonal closed packed structure to the face centred cubic structure takes place as size decreases to nanoscale. Deviation of the calculated model results from experimental values may be because we have not taken into account the crystal structures.

4. Conclusion

In this paper, we have studied the variation of magnetic properties of the nanomaterials with size and shape by considering three models, viz., Qi model, Jiang model and Lu model. It is found that Curie temperature (T_C), magnetisation (M_S) and Neel temperature (T_N) decreases with size of the nanomaterial. The anomalous nature of magnetic properties in nanomaterials is due to the change in surface to volume ratio with size and shape of the nanomaterial. The results calculated from Qi model are in good agreement with the available experimental data which validate the present work. Qi model works well for all the nanomaterials considered. It may be useful for the researchers who are engaged in the experimental analysis of magnetic properties of the nanomaterials.

References

[1] M Goyal and B R K Gupta, *Mod. Phys. Lett. B* **33**, 1950310 (2019)
[2] N Arora and D P Joshi, *Indian J. Phys.* **91**, 1493 (2017)
[3] S Bhatt and M Kumar, *Indian J. Pure Appl. Phys.* **56**, 210 (2018)
[4] W H Qi, *Physica B* **368**, 46 (2005)
[5] K Rawat and M Goyal, *High Temp.- High Press.* **49**, 279 (2020)
[6] G Guisbiers, *Adv. Phys. X* **4**, 1668299 (2019)
[7] S Bhatt, R Kumar and M Kumar, *Mod. Phys. Lett. B* **31**, 1750011 (2017)
[8] M Goyal and B R K Gupta, *Chin. J. Phys.* **56**, 282 (2018)
[9] H Chhabra and M Kumar, *Indian J. Phys.* **95**, 267 (2020)
[10] B Aktas, L Tagirov and F Mikailov, *Magnetic nanostructures* (Springer, Berlin, 2006)
[11] Y Li and T Wang, *J. Nanometer.* **2012**, 897203 (2012)
[12] B Sadeh, M Doi, T Shimizu and M J Matsui, *J. Magn. Soc. Jpn.* **24**, 511 (2000)
[13] X He, W Zhong, C T Au and Y Du, *Nanoscale Res. Lett.* **8**, 446 (2013)
[14] N J Tang, W Zhong, H Y Jiang, X L Wu, W Liu and Y W Du, *J. Magn. Magn. Mater.* **282**, 92 (2004)

[15] Q Meng, N Zhou, Y Rong, S Chen and T Y Hsu, *J. Acta Mater*. **50**, 4563 (2002)

[16] C Ling-fei, X Dan, G Ming-xing, H S Park and T Fujita, *Trans. Nonferrous Met. Soc. China* **17**, 1451 (2007)

[17] Q Jiang, X F Cui and M Zhao, *Appl. Phys. A* **78**, 703 (2004)

[18] E M Chudnovsky and L Gunther, *Phys. Rev. Lett*. **60**, 661 (1988)

[19] D D Awschalom and D P Divincenzo, *Phys. Today* **48**, 43 (1995)

[20] C Liu and Z J Zhang, *Chem. Mater*. **13**, 2092 (2001)

[21] H M Lu, W T Zheng and Q Jiang, *J. Phys. D* **40**, 320 (2007)

[22] W H Qi and M P Wang, *Mater. Chem. Phys.* **88**, 280 (2004)

[23] Q Jiang, H Y Tong, D T Hsu, K Okuyama and F G Shi, *Thin Solid Films* **312**, 357 (1998)

[24] H M Lu, P Y Li, Z H Cao and X K Meng, *J. Phys. Chem. C* **113**, 7598 (2009)

[25] X Y Lang, W T Zheng and Q Jiang, *Phys. Rev. B* **73**, 224444 (2006)

[26] L H Liang and B Li, *Phys. Rev. B* **73**, 153303 (2006)

[27] W H Qi, B Y Huang, M P Wang, Z M Yin and J Li, *Physica B* **403**, 2386 (2008)

[28] C C Yang and Q Jiang, *Acta Mater.* **53**, 3305 (2005)

[29] X G Zheng, C N Xu, K Nishikubo, K Nishiyama, W Higemoto, W J Moon, E Tanaka and E S Otabe, *Phys. Rev. B* **72**, 014464 (2005)

[30] E N Abarra, K Takano, F Hellman and A E Berkowitz, *Phys. Rev. Lett.* **77**, 3451(1996)

[31] W H Qi, M P Wang and Q H Liu, *J. Mater. Sci.* **40**, 2737 (2005)

[32] Q Jiang and X Y Lang, *The Open Nanosci. J.* **1**, 32 (2007)

[33] C Q Sun, W H Zhong, S Li, B K Tay, H L Bi and E Y Jiang, *J. Phys. Chem. B* **108**, 1080 (2004)

[34] A Kolhatkar, A Jamison, D Litvinov, R Willson and T Lee, *Int. J. Mol. Sci.* **14**, 15977 (2013)

[35] A Punnoose, H Magnone and M S Seehra, *Phys. Rev. B* **64**, 174420 (2001)

[36] R N Panda, Gajbhiye and G Balaji, *J. Alloys Compd* **326**, 50 (2001)

[37] W Gong, H Li, Z R Zhao and J C Chen, *J. Appl. Phys.* **69**, 5119 (1991)

[38] Z L Liu, Y J Liu, K L Yao, Z H Ding, J Tao and X Wang, *J. Mater. Synth. Process.* **10**, 83 (2002)

[39] D Alders, L H Tjeng, F C Voogt, T Hibma, G A Sawatzky, C T Chen, J Vogel, M Sacchi and S Iacobucci, *Phys. Rev. B* **57**, 11623 (1998)