Some Factors Affecting on Magnetic Characteristic Quantities and $T_c$ Curie Phase Transition Temperature of the Ni Nanoparticles by the Classical Heisenberg Model

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Abstract

This paper investigates the effect of particle size $D = 4.51$nm, $5.03$nm, $5.42$nm, $5.91$nm, rate of heat $4.10^{12}$K/s, $4.10^{13}$K/s, $4.10^{14}$K/s on magnetic characteristic quantities: Magnetization $M$, specific heat $C_v$, energy $E$, magnetic susceptibility $\chi$ and $T_c$ Curie phase transition temperature by classical Heisenberg model. The results show when increasing D particle size then $T_c$ Curie transition temperature increases and when increasing rate of heat then $T_c$ decreasing. In addition, there is the influence of D size and heating rate on magnetic characteristic quantities.

Keywords: influence, particle size, rate of heat, $T_c$, Curie transition temperature, classical Heisenberg model.

1. Introduction

Now, Ni nanomaterials are being used in the science, technology and biomedical. Optical catalysts [1], [2], photovoltaics [11], solar cells [3], [4]. To create the Ni nanoparticles, there are many methods. Chemical methods [5], [6], [7], physical methods [8], [9] and molecular dynamics simulation methods [30] and Monte Carlo method [31]. The results showed, $T_m$ phase transition temperature always proportional with N$^{1/3}$ atoms number [10], [11], [12], [13], [14], [15]. $T_p$ crystallization temperature of the nanowires always inversely proportional with D size [11] and $T_c$. Curie phase temperature be determined by semi-empirical formula give results smaller than 631K [16]. For size D = 24nm, 50nm, 96nm, 165nm, 200nm then $T_m$ = 593K, 612K, 622K, 626K, 627K and when D decreases then $T_m$ decreases [17], [18], [19], [20], [21], [22], [23], [24], [25], [26], [27], [28], [29]. In addition, there is also the effect of Ni nanoparticle size [49] and thin film thickness [50] on $T_c$ Curie transition temperature. Recently, investigated the effect of rate of heat, atomic number, temperature, and heating time on structure of Ni nanoparticles by Molecular Dynamics method with Sutton-Chen interaction, boundary conditions freedom [30] and characteristic quantities magnetic of Fe nanoparticles [31]. The results show, influence of D particle size on structure and magnetism. When increasing atomic number N lead to D particle size increases, proportional with N$^{1/3}$ and energy increases proportional with N$^{-1}$ [30] and appearance of BCC structure is interesting and controversial. With calculations based on analysis: Structural [45], [47] link angle analysis [46], link analysis [48] ... will solve this problem, $T_c$ Curie phase temperature increased [31]. In the article, influence of D particle size, rate of heat on magnetic characteristic quantities and $T_c$ Curie phase transition temperature of Ni nanoparticles.

2. Calculation Method

The study Ni nanoparticle with density $\rho$ and nanoparticle size evaluated by $D = 2 \left( \frac{3N}{4\pi\rho} \right)^{1/3}$

with $\rho = 7.72$ g.cm$^{-3}$. Inside N, V are atoms numbers total and volume of particle. Ni nanoparticles generated by molecular dynamics method with embedded interaction Sutton-Chen and free boundary condition [30]. The thermal processes follow law of Nosé el [43] and Hoover el [44]. To determine magnetic characteristic properties, considered each atom of Ni nanoparticle is an spin $S_r$, magnitude value of each spin is $|S_r| = 1$. Place Ni nanoparticles into classical Heisenberg model [32], [33], [34] with Hamilton function has form:

$$H = \sum_{\langle i, j \rangle_{BR}} J_{ij} (r_{ij}) (S_i \times S_j)$$

(2)

$\ln J_{ij} (r_{ij}) = J_0 \left( 1 + \frac{r_{ij}}{r_c} \right)^{-3}$

(3)

With $J_0$ is interaction energy between two nearest spins, $r_{ij} = |r_i - r_j|$ is shortest distance between two spins $S_i$, $S_j$ and $J_0$ is interaction energy between spins $S_i$, $S_j$ and $r_c = 3.35\\text{Å}$ is radius breaker. After that determining magnetic characteristics of nanoparticles Ni as:
\[ \langle E \rangle = \frac{1}{N} \langle H \rangle, \langle M \rangle = \frac{1}{N} \left| \sum S_i \right|, \]
\[ \langle C_v \rangle = N \frac{\langle E^2 \rangle - \langle E \rangle^2}{(k_B T)^2}, \langle \chi \rangle = N \frac{\langle M^2 \rangle - \langle M \rangle^2}{k_B T} \]

(4)

and \( T_c \) Curie phase transition temperature.

Inside, magnetic characteristic quantities has related to \( J_0 \) interaction energy which is currently unknown by theory model well as in empirical. used Moten-Carlo method, combined with error method of physical quantity measurement to determine \( J_0 \) by:

First, determining average value of \( \bar{T}_c = \frac{1}{N} \sum_{i=1}^{N} T_c \) and absolute error \( \Delta T_c = |T_c - \bar{T}_c| \) of Ni_{4000} nanoparticles with \( D = 4.51\text{nm} \) according \( J_0 = 0.4; 0.5; 0.6; 0.61; 0.63; 0.67; 0.69; 0.7; 0.8 \) and comparing obtained results \( T_c \) with results of semi-empirical formula \( T_{es} \) (5) and then selecting \( J_0 \) with minimum \( \Delta T_c \) absolute error.

\[ T_{es}(D) = T_{es} \exp \left( -\frac{2S_{sb}^2 1}{3R (D/6h-1)} \right) \]

(5)

With \( S_{sb} = 10.12 \text{J/mol.K}; h = 0.2492\text{nm}; T_{es} = 631\text{K}; R = 8.314 \text{J/mol.K} \) [35], [36], [37] have \( T_{es} \) of Ni nanomaterials. All of the nanoparticles were done with sufficient time to reduce statistical errors. Recovery time is \( 10^6 \text{MC steps/spin} \) and the average statistical time is \( 2.10^6 \text{MC steps/spin} \).

3. Results and Discussion

3.1. Effect of \( J_0 \) Exchange Energy

To determine \( T_c \) Curie phase transition temperature of Ni_{4000} nanoparticle [30] with different \( J_0 \) exchange energy values, resulting Table 1, Figure 1.

| \( J_0 \) | \( T_c(K) \) | \( \bar{T}_c(K) \) | \( \Delta T_c = |T_c - \bar{T}_c| (K) \) |
|---|---|---|---|
| 0.4 | 271.6 | | 131.7 |
| 0.5 | 339.5 | 403.3 | 63.8 |
| 0.6 | 400.6 | | 2.71 |
| 0.7 | 468.6 | | 65.3 |
| 0.8 | 536.4 | | 133.1 |

The results show, \( T_c \) Curie phase transition temperature has average value \( \bar{T}_c = 403.3\text{K} \) (table 1) and in range \( J_0 = (0.6; 0.7) \).

The detailed result shows \( J_0 = 0.63 \) has smallest absolute error (Figure 1). So, choose \( J_0 = 0.63 \), with neighborhood radius \( r_c = 3.35\text{Å} \) to study. This is method very useful for theory studies, empirical to determine \( J_0 \) values for a variety of materials.

3.2. Effect of \( D \) Particle Size

The results show, \( T_c \) Curie phase transition temperature has 3.35Å to study. This is method very useful for theory studies, empirical to determine \( J_0 \) values for a variety of materials.
The results show the have influence of D on E, M, C\textsubscript{v}, \chi. When D increases from D = 4.51nm to 5.91nm then E decreases from -0.0972eV to -0.1003eV (Fig. 2a); M decreases from 1 to 0 and curvature descending (Fig. 2b); C\textsubscript{v} reached extreme value at T\textsubscript{c}, height of peak increased from 1.79257 to 2.0118 (Fig. 2c); height of peak increased from 276.59 to 550.83 (Fig. 2d). The displays for each T values correspond to a value M, C\textsubscript{v}, E, in particular. The display values do not include errors because error value at point each has less than size of display value. When T < T\textsubscript{c} then the curvature of the magnetization curve M increases when increasing D (Fig. 2b), decreasing when T > T\textsubscript{c} and this is the basis for existence ferromagnetic phase transition on Ni nanoparticles.

In addition, the results of Fig. 2c, Fig. 2d show that extreme values of C\textsubscript{v} and \chi increase when D increases and confirmed that To Curie phase transition temperature of Ni nanoparticles is phase transition temperature of type 1. To the observe structure of Ni nanoparticles, used the visualization method (Fig. 2e-2i). The results show, nanoparticles are made up of FCC, HCP, BCC, Amor structures and assert there is no messy arrangement of Ni atoms but instead is an arrangement of atoms according to the definite structure. In Ni\textsubscript{5324} nanoparticle has the appearance of BCC structure, explained in the article [30]. When increase N atoms number leading to D increase and E decreases it shows has the influence of D nanoparticle size on Ni nanoparticle structure. To confirm the accuracy of results, compared results T\textsubscript{c} simulation with results of semi-empirical formula T\textsubscript{es} (5) [28], [29], [36], results in Table 2, Figure 3.
Table 2. Comparison \( T_c \) Curie phase transition temperature of simulation method and \( T_{es} \) Curie phase transition temperature of semi-empirical with different nanoparticle size.

<table>
<thead>
<tr>
<th>N Number (atoms)</th>
<th>4000</th>
<th>5324</th>
<th>6912</th>
<th>8788</th>
</tr>
</thead>
<tbody>
<tr>
<td>D Size (nm)</td>
<td>4.51</td>
<td>5.03</td>
<td>5.42</td>
<td>5.91</td>
</tr>
<tr>
<td>( T_c ) (simulation)</td>
<td>421 ± 3</td>
<td>448 ± 2</td>
<td>461 ± 4</td>
<td>475 ± 6</td>
</tr>
<tr>
<td>( T_{es} ) (semi-experimental formula) [28], [29], [36]</td>
<td>425</td>
<td>448</td>
<td>463</td>
<td>479</td>
</tr>
</tbody>
</table>

Figure 3. The relationship between \( T_c \) Curie phase transition temperature of simulation method and \( T_{es} \) Curie phase transition temperature results of semi-empirical formula with different nanoparticle sizes.

The results show, with each value of D will have \( T_c \) and \( T_{es} \) respectively. To evaluate error at each value \( T_c \) and \( T_{es} \) use the interpolation method. These results showed, table 2 including \( T_c \) value respectively, error value at each point and \( T_{es} \) is determined by semi-empirical formula (5) to the comparison. Here determined the relationship between \( T_c \) and \( T_{es} \): \( T_{es} = T_c ± (2 \text{ or } 6) \text{ K} \) with D increased from 4.51 nm to 5.91 nm. After comparing results between \( T_c \) and \( T_{es} \) [28], [29], [36] (Fig. 3) show results has duplication. The simulated results show that it is not only consistent with results of semi-empirical formula but also good fit with simulation results of bulk material and thin films [29], [38], [39], [41], [42], [49], [50] the value obtained within allowable limit and confirmed by influence of D on magnetic characteristic quantities and \( T_c \).

3.3 Effect of Heating Rate

To study magnetic characteristics and \( T_c \) Curie phase transition temperature at different structural states corresponding with different heating rates results in Figure 4.
The results show, when increased rates of heating from 4.10^{12} K/s to 4.10^{14} K/s then energy increased (Fig. 4a), magnetization decreases (Fig. 4b), specific heat is constant (Fig. 4c) while magnetic susceptibility changes to negligible (Fig. 4d). When heating rate increases lead to $T_N$, Curie phase transition temperatures decreases it shows Ni nanoparticles have moved on the amorphous state. Results structural change from crystalline state to the amorphous state leading to energy increased. The structural shape results (Fig. 4e-4h) shown HCP, FCC structural unit number decrease, and Amor increase is 93.98%. These results are consistent with the results shown in Figure 4a-4d and very useful for studying structure and magnetism of Ni nanoparticles.

4. Conclusion

Study on effect of particle size, the heating rate on magnetic characteristic and Curie $T_N$, phase transition temperature of Ni nanoparticles, results obtained: Successful determination of nanoparticle exchange energy is 0.63. When nanoparticle size increased lead to $T_N$, Curie phase transition temperature increased, results were consistent with article [28], [29], [36]. When heating rate increases lead to structure changes from crystalline state to the amorphous state resulting $T_N$ decrease. This is due to the structural change from crystalline state to the amorphous state leading to energy increased. The simulated results show it is not only consistent with the results of the semi-empirical formula but also consistent with results of bulk material and thin films [29], [38], [39], [41], [42], [49], [50].

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References


