Hysteresis in Core/Shell Nanowire with Mixed Spin Ising

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Abstract

In this work, Monte Carlo simulations (MCS) based on Metropolis algorithm were performed to study the hysteresis loops and coercive field of a core/shell nanowire with spins $S = \pm \frac{5}{2}, \pm \frac{3}{2}, \pm \frac{1}{2}$ and $\sigma = \pm \frac{3}{2}, \pm \frac{1}{2}$, respectivevility, considering an Ising ferrimagnetic system. The influence of nearest neighbors exchange interactions and crystal field anisotropy on hysteresis and coercive field behaviors of the system has been analyzed. The calculations were performed using a single-spin flip algorithm. In each spin-flip attempt, we randomly choose a site. The results show that, for a system without anisotropy triple hysteresis loops appear for certain values. The plateaus in hysteresis loops are due to the values of the spins projections. The change of the values for anisotropy influence the shape of the hysteresis loops without present triple hysteresis loops. Also, the effect of the anisotropy in the coercive field was analyzed, where the coercive field present enhanced for certain range of the temperatures. Finally, for high values of the applied external magnetic field, the Zeeman effect takes control over the system.

Keywords: Monte Carlo method, core/shell nanowire, hysteresis loops, coercive field, ferrimagnetic system
1 Introduction

In recent years, magnetic nanostructures as nanoparticles systems, especially, magnetic nanowires, are currently increased the interest of theoretical and experimental researches, because of their fascinating properties, compared with other bulk materials [32]. In particular, the nanowires have been receiving considerable attention, experimentally, due to their distinctive properties for being used as ultrahigh magnetic recording media [20, 6]; they also have potential biotechnological applications as [22], [34] tissue targeting or hyperthermia [2], sensors [1] and medical applications [21], among others. On the other hand, core/shell nanotube (nanowire or nonorod) systems have been attracting for several technological applications as sensing, batteries and fuel cells. In particular, the properties of these arrays are strongly dependent on the interface between the materials used for building the core and shell [25]. Regarding to magnetic applications, several core/shell nanowires can exhibit different functionalities. For instance, systems formed by combinations of materials as ferromagnetic core and antiferromagnetic shell, different ferromagnetic materials for core and shell, ferromagnetic core and antiferromagnetic shell, among others, can enhance unidirectional anisotropy, magnetic resonance and generate special properties as exchange bias [18]. Studies of core/shell nanoparticles have revealed interesting magnetic properties, such as tuning of the blocking temperature with four-fold increase in the coercivity [30], optimized hyperthermia [23] and enhanced coercitivy [5].

Theoretical studies have shown that this mixed system has an interesting magnetic behavior, with several compensation temperatures, tri-critical points and reentrant behavior [26], [7]. The possible applications in the design of new materials motivate the study of nanoparticles with high spin values. The behavior of hysteresis has been investigated for cylindrical nanowires within the effective-field theory (EFT) varying the interaction (ferromagnetic and antiferromagnetic) [17]. Also, it has been studied the behavior of hysteresis and compensation in cylindrical Ising nanotube systems. Kocakaplan et al., [17] observed that areas of hysteresis loops decrease as the temperature increases and disappears at certain temperatures. Also, showing the different forms that hysteresis loops can exhibit. Using Monte Carlo simulations (MCS) hysteresis loops for core/shell nanoparticles have modeled [15]. A similar work was reported by A. Patsopoulos et al [28], that presented MCS for studying Co/CoO core/shell nanowires. In some cases, with certain conditions, a triple hysteresis loops were observed, in different systems, such cylindrical transverse spin $-1$ Ising nanowire [19] and spin $-1/2$ cylindrical Ising nanowire with a core/shell structure [17].

In the literature, other interesting works presenting Monte Carlo simulation of core/shell nanostructures can be found; for instance, Eftaxias and
Trohidou [8] used Monte Carlo simulations for studying the exchange bias and coercive field of nanoparticles with ferromagnetic and antiferromagnetic core and shell, respectively. They found a strong dependence between these parameters, and the structure and size of the interface. They also found a good agreement with experimental reports. Zaim and Kerouad [35] performed a Monte Carlo simulation of magnetic properties of spherical nanoparticles, consisting of ferromagnetic core and shell with spins $S = \pm 1/2$ (core) and $\pm 1.0$ and $S = \pm 1/2, \pm 3/2$ (shell), with antiferromagnetic interface coupling. They found that, for appropriated values of the system parameters, two compensation temperatures can be occurred in the system. Vasilakaki et al [33], employed the Monte Carlo method for studying the exchange bias effect at an atomic level; they also observed a training effect in ferromagnetic/antiferromagnetic core/shell nanoparticles. Moreover, they analyzed the effect of the dipolar interaction between particles, also included a study of the hysteresis loop behaviors. Estrader et al [11], presented a study of magnetic behavior of bi-magnetic hard-soft, core/shell nanoparticles. They used experimental techniques as magnetometry, ferromagnetic resonance and X-ray magnetic circular dichroism. They also performed Monte Carlo simulations for proving the consistency of the AFM coupling. More recently, Cansizoglu et al [4], analyzed vertical aligned in core/shell nanowire (nanorod) arrays; they concluded that, this geometry favors the construction of several nano-scale devices for new energy solar, sensor, detectors and spintronics. For this reason, they conducted experimental works using physical vapor deposition techniques and, as a complement, they carried out Monte Carlo simulations to estimate the best deposition technique for a conformal shell coating. Finally, Belhaj et al [3], published a study of the magnetic behavior of a nanostructure based on a hexagonal core (spin $\sigma = -3/2$) shell geometry (spin $S = 2$). Exactly, they are focused on determining the effect of the coupling exchange interactions on the absence/presence of both, an external magnetic and crystal fields. As an important result, they found a compensation temperature between the spins $\sigma$ and $S$. They also included a study of the hysteresis loop behaviors.

More recently studies with MCS in hexagonal ferrimagnetic Ising nanowire [12], Blume Capel model [29] and Quantum Monte Carlo [13] show the appearance of plateaus and different forms of hysteresis loops. However, mixed spin core/shell systems have been less investigated. For this reason, it is necessary to devote attention in these kind of systems. In this work, we study the effect of the crystal field and the exchange interactions on the coercive field, presenting triple hysteresis loops that disappear at high temperatures. The aim of this paper is to model hysteresis loops behavior of core/shell nanowire with spins $\pm \frac{5}{2}$ and $\pm \frac{3}{2}$ using Monte Carlo simulations. The outline of this paper is the following: In Section 2, we give the model and method of the Monte Carlo
simulations. In section 3, we present the results of the hysteresis loops and relationship coercive field and temperature. Finally, the conclusions are given in Section 4.

## 2 Model and Method

We consider a mixed spin Ising system composed by a core/shell nanowire with spins $S = (\pm \frac{5}{2}, \pm \frac{3}{2}, \pm \frac{1}{2})$ and $\sigma = (\pm \frac{3}{2}, \pm \frac{1}{2})$, respectively. The schematic representation of the cylindrical Ising nanowire is illustrated in Fig 1a. This Figure consists of a ferromagnetic core and shell with an anti-ferromagnetic coupling between core and shell, in which, the core is surrounded by the surface shell, where $r$ and $R$ are core and shell radii, respectively, with height $h$. The Fig 1b shows a represent the values of spins by means of arrows. Periodic boundary conditions were imposed in the $z$ direction. To study the magnetic behavior. The Hamiltonian includes terms as exchange interactions, crystal field anisotropy and the Zeeman effect, described by equation (1):

$$
\mathcal{H} = -J_{cc} \sum_{\langle i,j \rangle} S_i S_j - J_{ss} \sum_{\langle i,j \rangle} \sigma_i \sigma_j - J \sum_{\langle i,j \rangle} \sigma_i S_j - K_v \left( \sum_i \sigma_i^2 + \sum_j S_j^2 \right) - H \left( \sum_i \sigma_i + \sum_j S_j \right)
$$

where $J_{cc}$ and $J_{ss}$ are the exchange constants between the core-core and shell-shell, $J$ is the constant of exchange representing the anti-ferromagnetic coupling and, for this case, it is defined as $-1$. $S$ and $\sigma$ correspond to the spins of core and shell, respectively. The sum over $\langle i,j \rangle$ indicates that interaction is only taken into account between near neighbors; $K_v$ is the magnetocrystalline anisotropy constant and finally, $H$ is the external magnetic field, that is applied to the sample in the direction $z$. Error bars were obtained from averaging a number of 5 runs for each configuration, using different seeds for the random numbers.
The simulations were performed using Metropolis dynamics with 30000 Monte Carlo steps; where the first 10000 steps were discarded for the relaxation. The magnetizations of the two subsystems were found through:

\[ M_c = \frac{1}{N_c} \sum_i S_i \]

\[ M_s = \frac{1}{N_s} \sum_i \sigma_i \]

where \( N_c \) and \( N_s \) indicate the number of sites of the core and shell, respectively. The total magnetization comes given for:

\[ M_t = \frac{N_c M_c + N_s M_s}{N_c + N_s} \]

Hysteresis loops were performed by cycling the magnetic field from \( H = 25 \) to \(-25\) in steps of 1 by performing 30000 Monte Carlo steps per spin. The coercive field is defined as:

\[ H_c = \frac{H_{right} - H_{left}}{2} \]

where \( H_{right} \) and \( H_{left} \) are the points of the loop that intersect the field axis.

3 Results and Discussion

The results of this work are focused on analyzing the behavior of the hysteresis loops and coercive field of core/shell nanowires, below and around of the critical temperature and the compensation temperature. In a previous
work, the behavior of critical and compensation temperatures of the core-shell nanowires was studied [16], based on this work, the appropriate parameters were chosen for the simulations, where compensation temperature \( T_{\text{comp}} \) was observed and there was identified a difference between the compensation and the critical points.

### 3.1 Exchange interactions

The magnetic hysteresis loops for \( M_{\text{core}} \), \( M_{\text{shell}} \) and \( M_{\text{total}} \) at different reduced temperatures \( (T = k_B T/|J|) \) below and around the critical value, in the absence of the crystal field are calculated and plotted in Figure 2 at different temperatures \( (T_e = 1.5, 5.5, 10.5 \text{ and } 16.0) \) for \( J_{cc} = 0.8 \), \( J_{ss} = 4.0 \) and \( K_v = 0.0 \). From this result, it is observed that, when the temperature increases, the area of the hysteresis loops decreases, since the paramagnetic phase is reached. In addition, at low temperatures, plateaus appear, and then, they disappear with the increase of the temperature, close to the critical value. This result is in good agreement with the cylindrical Ising nanowire that has been investigated within the effective-field theory with spin \( \pm 1 \) [17] and the cylindrical nanotube system with spin \(-3/2\) [17]. Figure 2a shows a hysteresis loops at \( T_e = 1.5 \); for \( M_{\text{core}} \), triple hysteresis loops appear, while in the case of \( M_{\text{shell}} \) and \( M_{\text{total}} \), a unique internal area is observed, but including some plateus formation. The plateus represent the values of the possible projections of the spins. The Figure 2b with \( T_e = 5.5 \) triple hysteresis loops appear for \( M_{\text{total}} \); as is observed, the number of plateaus decreases. This behavior is due to, as the temperature increases, less field is required to reach the spins reversion process; then, the Zeeman effect dominates the system. In Figure 2c hysteresis loops for \( T_e = 10.5 \) were obtained, where it is presented a single cycle of the hysteresis for all the magnetizations. Finally, cycles obtained at \( T_e = 16.0 \) are shown in Figure 2d, where curves exhibit only a unique central loop. For the four cases, it was observed that, \( M_{\text{core}} \) presented more significant changes regarding to the form of the cycle. On the other hand, \( M_{\text{shell}} \) remains almost the same form (square), for all the temperatures analysed here, but varying the area. The behavior of the shell magnetization resembles a typical ferromagnetic material, while \( M_{\text{total}} \) strongly changes with the increase of the temperature. The changes of \( M_{\text{total}} \) are mainly affected by \( M_{\text{core}} \). Calculations were made changing the values of the projections for the core and shell; and it was found that the magnetizations behave the same. The plateaus in \( M_{\text{core}} \) were due to different possible projections of the spins. With the change in temperature, the transitions tend to become more gradual, and the cycles are smoothed, until above the system becomes paramagnetic and the hysteresis disappears. Also, a term is added that corresponds to the thermal fluctuations.

In all the Figures the arrows that indicate the changes in the projections
of the spins are shown, which explains the existence of the plateaus in the cycles of hysteresis. As the temperature used for the hysteresis cycle increases, the cycle softens and the plateaus stop appearing. In general, for the core magnetization, the most notable changes are presented, for which it is controlled the form of the hysteresis cycle for $M_{\text{total}}$. In the case of the $M_{\text{shell}}$ the changes of the projections are similar in all cases, this is due to the value of the spin that was given to this subsystem, the shape of the cycle resembles the behavior of a ferromagnetic material, since the coupling between core-core ions is a ferromagnet. For $M_{\text{total}}$, in all cases, all the possible projections of the spins appear, with the increase in temperature changes the number of plateaus in the cycles. At low temperatures, the number of plateaus is greater, because the zeeman effect still does not dominate the system, as happens when higher temperature is used. With the increase of the temperature, decreases the area of the cycle. In Figure 2a, for $M_{\text{core}}$ and $M_{\text{total}}$, all the projections of the spins appear, because they take all the possible values due to the temperature that was used. In Figure 2b a triple hysteresis loop with the central loop appears; similar results appear for the double-walled cubic nanotube [10]. For Figure 2c, the cycle of hysteresis is smoothed and all projections continue to appearing, obtaining a simple hysteresis cycle. In Figure 2d, the temperature that is approaching the critical temperature was used and its area is shrinking, appearing a central cycle. Multiple hysteresis loops have also been found, theoretically, in a mixed spin $-1$ and spin $-3/2$ core/shell cubic nanowire [24] and in CoFeB/Cu,CoNiP/Cu,FeGa/Py and FeGa/CoFeB multilayered nanowires [31].
Figure 2: The hysteresis loops at different reduced temperatures which are around the critical temperature with $T_c = 16.153$, $J_{cc} = 0.8$, $J_{ss} = 4.0$ and $K_v = 0.0$ a) $T_e = 1.5$ b) $T_e = 5.5$ c) $T_e = 10.5$ and d) $T_e = 16.0$. 
3.2 Magnetocrystalline Anisotropy

Figure 3: The hysteresis loops at different reduced temperatures which are around the critical temperature with $T_c = 19.6435$, $J_{cc} = 0.1$, $J_{ss} = 4.0$ and $K_v = 15.0$ a) $T_e = 0.5$ b) $T_e = 4.0$ c) $T_e = 7.5$ and d) $T_e = 13.0$. 
Figure 3 shows the hysteresis loops for $M_{\text{total}}$, $M_{\text{core}}$ and $M_{\text{shell}}$, respectively, at $T_e = 1.0, 4.0, 7.5$ and $13.0$, for $J_{cc} = 0.1, J_{ss} = 4.0$ and $K_v = 15.0$. For all cases, the same behavior that for $K_v = 0.0$ was observed. Figure 3a shows the cycle at $T_e = 1.0$, where plateaus for $M_{\text{total}}$ and $M_{\text{core}}$ appear. The arrows represent the spin projections. For $M_{\text{total}}$ only the projections for spins $\pm \frac{5}{2}$ and $\pm \frac{3}{2}$ appear, presenting a triple hysteresis loop. There is no evidence of the presence of spin $\pm \frac{1}{2}$, because in this point, the energy of the system is high. Respect to $M_{\text{core}}$, in the hysteresis loops, only the projections for $\pm \frac{5}{2}$ were observed. Moreover, $M_{\text{shell}}$ only presents values for $\pm \frac{3}{2}$. The presence of plateaus is produced due to the changes of the hysteresis loops because of the spins projection, that are represented by means of arrows. Figure 3b, developed at $T_e = 4.0$, shows the same projections for the three cases of the magnetizations at a temperature of $T_e = 1.0$. Regarding Figure 3c, a single cycle with a central hysteresis loop is presented for $M_{\text{total}}$. In the case of $M_{\text{core}}$, the cycle becomes thinner, because it is close to the critical temperature. In Figure 3d, for $M_{\text{total}}, M_{\text{shell}}$ and $M_{\text{core}}$, the spin projection $\pm \frac{1}{2}$ can be observed. In this point, the energy is minimized by increasing the temperature. In Figure 3c a smoothed loop was observed at $T_e = 7.5$, decreasing the area of the cycle, having the same behavior of the curve presented in Figure 3a and Figure 3b, where the projections were $\pm \frac{5}{2}$ and $\pm \frac{3}{2}$. In Figure 3d, for $M_{\text{core}}$, two jumps appear; these jumps are due to the projections $\pm \frac{1}{2}$ in $M_{\text{shell}}$. For the case of $M_{\text{total}}$, a central cycle appears, because of the high temperature applied. The effect of the magnetocrystalline anisotropy was a phase transition that happens at higher temperature. The hysteresis loop forms were not affected when $K_v$ is included.

### 3.3 Coercive Field

The coercive field is the ability of a material to resist the magnetic field without demagnetizing. In this section, the behavior of the coercive field is presented as a function of the temperature for the core, the shell and the total system, considering variations of $J_{cc}$, $J_{ss}$ and $K_v$.

#### 3.3.1 Shell Coercive Field

Figure 4 shows shell coercive field as a function of the temperature for a) $J_{ss} = 4.0$ and $K_v = 0.0$ varying $J_{cc}$, b) $J_{cc} = 0.1$ and $K_v = 0.0$ varying $J_{ss}$ and c) $J_{ss} = 4.0$ and $J_{cc} = 0.1$ varying $K_v$. In Figure 4a, the changes with respect to $J_{cc}$ were presented; in the four cases, the curves were overlaped, indicating that $M_{\text{shell}}$ takes the same values of $H_c$. Therefore, for the coercive field, the changes in $J_{cc}$ values do not affect its behavior, because a similar critical temperature is maintained for the values $J_{ss}$ and $J_{cc}$ used in these cases. In Figure 4b, the coercive field curves tend to decrease, exhibiting same behavior than in the case of Figure 4a; nevertheless, in this case the curves
are not overlaped, as $J_{ss}$ is increased. An increase in the values of coercive field is observed, due to $T_c$ moves towards the right, as $J_{ss}$ increases. This phenomenon was explained in preliminary works, where it was found that, the increase in the critical temperature should be maintained periodic with the periodic variation of $J_{ss}$ [16]. In Figure 4c, as $K_v$ increases, the same behavior as it obseved in figure 5a appears. As it was previously observed (In section 3.2) it does not affect the shape of the cycles; it only imposes more order in the system.

On the other hand, the coercive field tends to zero, as the temperature increases, as is expected for a typical ferromagnetic material. The shell and the core are considered as independent systems for the analysis of $H_c$.

3.3.2 Core Coercive Field

Figure 5, shows the core coercive field as a function of the temperature for a) $J_{ss} = 4.0$ and $K_v = 0.0$ varying $J_{cc}$, b) $J_{cc} = 0.1$ and $K_v = 0.0$ varying $J_{ss}$ and c) $J_{ss} = 4.0$ and $J_{cc} = 0.1$ varying $K_v$.
\(J_{ss}\) and c) \(J_{ss} = 4.0\) and \(J_{cc} = 0.1\) varying \(K_v\). Figure 5a presented the coercive field varying \(J_{cc}\). It is observed that, for \(J_{cc} = 0.2, 0.4\) and 0.6, the same behavior is presented. At low temperatures, \(H_c\) decreases from 0.5 down to 0, reaching a minimum point \(T < 2\); then, as the temperature increases, \(H_c\) increases up to values around 0.5; on the other hand, For \(J_{cc} = 0.8\), \(H_c\) starts at a high value (in the order of 2.5), reaching a minimum point, similar to the other cases, but at around at a temperature of 5. This is due to the fact that, for low relations between \(J_{ss}\) and \(J_{cc}\), the behavior of the \(H_c\) of the core respect is very variable due to the number of ions and the value of projections that are taken. In the Figure 5b all behave the same starting at the same values and reaching the maximums of \(H_c\), which move to the right with the increase of the \(J_{ss}\). The displacement is due as \(J_{ss}\) varies the \(T_c\) increases, and for low values the phase transition occurs first. For Figure 5c a behavior equal to Figure 5b is presented, in this case the behavior is due to the fact that when \(K_v\) is included in the system, the phase transition is made at a higher temperature, so the maximum is displaced. Unlike the case of the shell in this, there is an improvement in the coercive field that is due to the combination of the values of \(J_{ss}\) and \(J_{cc}\), accompanied by the values of the projections of the spins, which cause the hysteresis loops to vary constantly by increasing the temperature used for each cycle.
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3.3.3 Total Coercive Field

Figure 6 shows a total coercive field as a function of the temperature for a) $J_{ss} = 4.0$ and $K_v = 0.0$ varying $J_{cc}$, b) $J_{cc} = 0.1$ and $K_v = 0.0$ varying $J_{ss}$ and c) $J_{ss} = 4.0$ and $J_{cc} = 0.1$ varying $K_v$. Figure 4a, shows a similar behavior in all cases, for $J_{cc} = 0.2$ $H_c$ starts at low values (around 0.1) and then it increases; however, for $J_{cc} = 0.4 ,0.6$ and $0.8$, $H_C$ begins at a high value (around $0.9, 1.8$ and $3.0$, for $J_{cc} = 0.4 ,0.6$ and $0.8$, respectivility), decreasing and reaching its maximum as he temperature increases. The maximum value of $H_c$ exhibits a shift towards the right with the temeprature. This point, corresponds to $T_{comp}$ for this combination of $J_{cc}$ and $J_{ss}$. In this case of the Figure 4b the opposite case is presented to Figure 4a, all starts at low values and increases with the step of temperature, where appear a shift toward the right of the first point where $H_c = 0.0$, because $T_{comp}$ is different for each value of $J_{ss}$. For figure 4c, at temperatures lower than the critical value, $H_c$ exhibis similar behaviour and values; since in this region the effect the order of the system is controled by
the temperature; nevertheless, for $T > T_c$, the magnetocrystalline anisotropy, $K_v$, dominates the system ordering; then, as $K_v$ increases, the transition point is shifted toward greater temperature values, but remaining the shape of the four curves similar.

Table 1 shows the maximum values of $H_c$, varying $J_{cc}$, $J_{ss}$ and $K_v$. In figure 6a, varying $J_{cc}$, as the temperature increases, the maximum of $H_c$ tends to shift toward lower temperature. By varying $J_{ss}$, the maximum of $H_c$ increases, and it is shifted toward higher temperatures. On the other hand, varying $K_v$ the maximum value of $H_c$ remains almost constant, but a little increase in the temperature was observed. These changes in the values of $H_c$ and $T_c$ are due to the combination of $J_{ss}$ and $J_{cc}$. The study of the changes in $T_c$ was previously carried out, considering different values for $J_{ss}$ and $J_{cc}$ [16]. In all cases there is an enhancement of $H_c$, which has been evidenced in previous studies conducted in nanowires by means of Monte Carlo simulations [27, 9, 14].

Figure 6: Total coercive field in function of the temperature a) $J_{ss} = 4.0$ and $K_v = 0.0$ varying $J_{cc}$, b) $J_{cc} = 0.1$ and $K_v = 0.0$ varying $J_{ss}$ and c) $J_{ss} = 4.0$ and $J_{cc} = 0.1$ varying $K_v$. 
4 Conclusion

We employed Monte Carlo simulations to study the hysteresis behaviors of a core/shell ferrimagnetic nanowire with a mixed spin Ising spins $-5/2$ and $-3/2$. The influence of the exchange interactions and the crystal field on the behavior of the hysteresis loops, and coercive field was analysed. Results showed that the shape of the hysteresis cycles depends on the combination of the magnetic exchange constants. For the case of $J_{ss} = 2.0$ and $J_{cc} = 0.4$, triple hysteresis loops were presented. Because of the temperature, $H_c$ exhibited changes at around $T_c$. The enhancement of $H_c$ is favored at small $J_{ss}$ and large $J_{cc}$. When the magnetocrystalline anisotropy was included, a maximum was observed, and a greater value of this maximum can be found at $K_v = 0.0$; then, in can be concluded that the anisotropy does not favor the coercive field.

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