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Simulating magnetic nanotubes using a chain of ellipsoid-rings model with magnetization reversal process by fanning rotation

[a]Jieqiong Wang, [a]Sen Yang*, [a]Junfeng Gong, [a]Minwei Xu, [a]Murtaza Adil, [a]Yu Wang, [a]Yin Zhang, [a]Xiaoping Song, [b]Hao Zeng

Recently, magnetic nanotubes have attracted great attention owing to the advantages of tubular geometry. Of all the physical properties of magnetic nanotubes, the magnetic behavior plays a pivotal role in the potential applications, particularly in biotechnology. Modeling magnetic nanotubes provides an effective way to obtain the geometry dependent magnetic properties. In the present article, we model the nanotube as a chain of ellipsoidal-ring; thus the magnetic behavior of nanotubes is simulated by fanning rotation of magnetic moments. Based on this model, we further discuss the influence of tubular geometric parameters on the magnetic properties. The calculated magnetic properties of Fe, Co, Ni, Fe_3O_4 and $CoFe_2O_4$ nanotubes which are all well consistent with their experimental data. Consequently, our model provides an easy and general approach to magnetic nanotubes.

1.Introduction

For the past decades, magnetic nanostructures (particles, films or wires in the nanoscale) have attracted increasing interest due to their interesting properties and potential applications in various fields, such as ultrahigh-density data storage, magnetic resonance imaging, magnetically guided drug delivery, and so on [1-13]. To apply these magnetic nanostructures in practical devices or architectures, the size-tunable nanostructures are desired to fit for the working circumstances. For instance, a drug delivery system requires its magnetic nanostructure, a vehicle to convey the drug guided by magnetic field, to vary the size and shape in more geometric parameters for *in vivo* application [14,15]. The nanoparticle preferentially possesses spherical shape but leaves only one geometrical parameter, the radius of the sphere to modify; the nanowire can change both length and radius of wire, but its application is greatly limited due to its solid construction (e.g. it cannot be used for drug delivery). Thus, a tubular structure that could vary the both hollow inside would be highly desirable in the development of nanostructures [15].

Compared to magnetic nanowires, magnetic nanotubes have caused extensive attentions owing to their advantages of tubular geometry, where the magnetic properties of nanotube can be adjusted by varying an additional geometric parameter of wall thickness besides length and radius. Furthermore, other materials can be deposited inside the hollow tubes by chemical/physical processes to form core/shell nanostructures, resulting in prospective applications [6-13,16,17], particularly in biotechnology such as imaging[17] and drug delivery[15]. For the research of magnetic nanotubes, the key issue is to fully understand the change of magnetic properties with the geometric parameter of nanotubes. Although the magnetic properties of nanotubes have been extensively

[a]*School of Science, MOE Key Laboratory for Nonequilibrium Synthesis and Modulation of Condensed Matter, State Key Laboratory for Mchanical Behavior of Materials. Collaborative Innovation Center of Suzhou Nano Science and Technology, Xi'an Jiaotong Universiy, Xi'an 710049, China*

[b]*Department of physics, University at Buffalo, the State University of New York, Buffalo, NY14260, USA*

E-mail: yangsen@mail.xjtu.edu.cn; Tel: +86-29-82668302

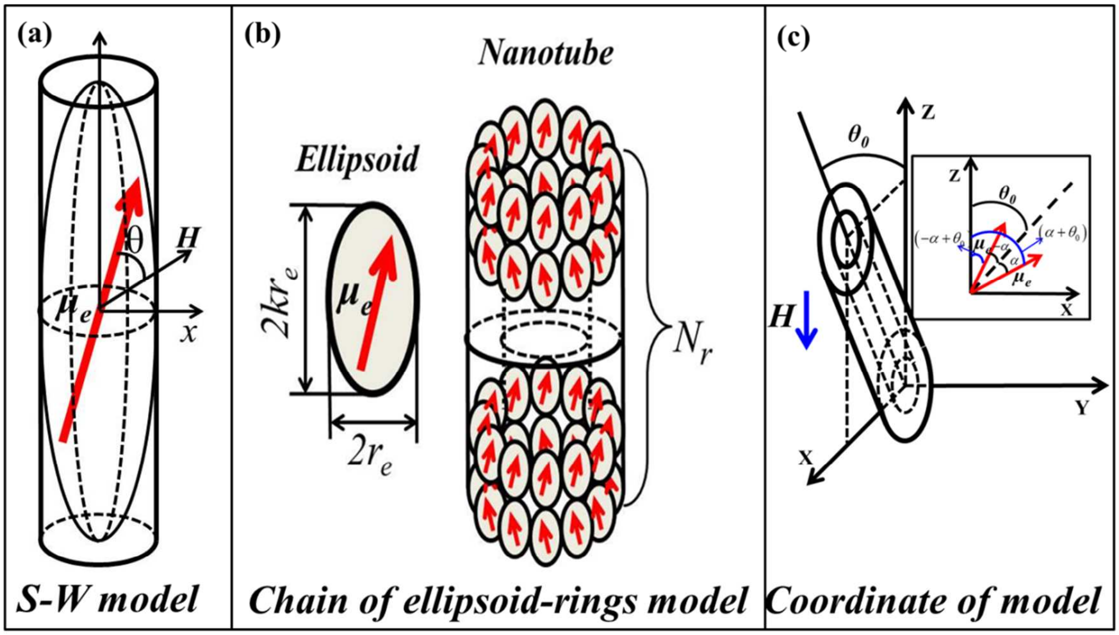

Fig.1Schematic diagram of models used for the calculation of magnetic properties of nanotubes (a) Stoner-Wohlfarth (S-W) model. (b) The chain of ellipsoid-rings model with fanning reversal mechanism. (c) Coordinate of the model of chain of ellipsoid-rings.

investigated by experiments [19-22], the geometric parameter dependence of magnetic behavior remains a challenging task; this is mainly due to that the synthesis of magnetic nanotubes is confined in a limited geometric range. To investigate the magnetic properties in a whole range of tubular geometry and guide the synthesis of the magnetic nanotubes, an appropriate model for the calculation of magnetic properties of nanotubes becomes crucially important**.**

Currently, most theoretical studies of magnetic properties of nanotubes are mainly on the Stoner-Wohlfarth (S-W) model [23], where the nanostructure is considered to be an elongated prolate-ellipsoid with a single domain, as schematically shown in Fig. 1(a). Although such a model has been successfully employed to simulate the magnetic properties of nanotube and furthermore some results of simulation are partially consistent with experimental results, an elongated prolate-ellipsoid with solid construction in S-W model heavily deviates from the real geometry of hollow tubular structure; hence the realization of predicted magnetic properties by S-W model has been hindered by the experimental difficulties.

Very recently, according to the geometric feature of nanotube, we set up a chain of ellipsoid-rings model to simulate the magnetic behavior of nanotubes and obtained results consistent with the experimental measurement, e.g. in Ni nanotubes [24]. As the magnetic properties are tightly related to the rotation of magnetic moments, the magnetization reversal process plays a key role to simulate the magnetic nanotube. There are several magnetization reversal processes in the rotation of magnetic moments, including coherent, fanning, curling and buckling rotation [25,26]. It is interesting to note that simulating magnetic nanotube by using of same model but different magnetization reversal processes might lead to different results; therefore, to fully understand the magnetic behavior of nanotubes, it is worth studying the magnetic properties with different magnetization reversal processes. In our previous work, with the coherent rotation of magnetic moments, we have simulated the magnetic nanotubes by a chain of ellipsoid-rings model. In the present article, we demonstrate an alternative magnetization reversal process of fanning rotation in the model of chain of ellipsoid-rings to theoretically investigate the magnetic behavior of nanotubes. Based on fanning rotation, we calculate the angular dependence of magnetization reversal process in the nanotubes and systematically discuss the influence of nanotube geometric parameters on the magnetic behavior of nanotubes; such parameters include the axial ratio of single ellipsoid (k), number of rings (N_r) and wall thickness ratio of the tube ($\Delta R/R$). Finally, we discuss the fanning rotation and coherent rotation in the ellipsoid-rings model, and then compare it with the S-W model. In addition, we draw a comparison between the calculated coercivity value and the experimental data of Fe, Co, Ni, Fe_3O_4 and $CoFe_2O_4$, and report the optimum k value for each specific magnetic nanotubes.

2. Model

2.1 Description of a chain of ellipsoid-rings model with magnetization reversal process by fanning rotation

Figure 1(b) schematically shows the structure of a chain of ellipsoid-rings model with magnetization reversal process by fanning rotation. In this model, a single nanotube is considered as a chain of rings and each ring is composed of ellipsoids with the major axis along the direction of tube axis, in which the number of rings and the number of ellipsoids in a ring are N_r and N_e, respectively. In order to keep magnetically isolated, all the ellipsoids in the nanotubes are assumed to have only point contact or even to be slightly separated. Thus, the contribution of wall energy of tube to the total magnetic energy becomes insignificant and, hence, can be omitted in the calculation.

All ellipsoids are assumed to have the same parameters, and hence, we define the radius of the minor and major axis of an ellipsoid as r_e and kr_e (k is the axial ratio of an ellipsoid), respectively. Thus, the wall thickness (ΔR) of the nanotubes is equal to $2r_e$. A special case is that the axial ratio (k) is equal to unity and correspondingly an ellipsoid becomes a sphere and its shape anisotropy disappears. For simplicity, each ellipsoid is treated as a dipole of magnetic moment $\boldsymbol{\mu_e}$. Thus, during the magnetization reversal process with fanning rotation of magnetic moments, all the dipoles of ellipsoids in the same ring rotate to one direction, while the dipoles in the neighboring rings rotate to the opposite direction, looking like a fan as shown in Fig. 1(b).

2.2 Exchange energy E_{ex}, Zeeman energy E_{ze} and anisotropy energy E_{an}

Simulating the properties of magnetic nanotube starts from the calculation of magnetic energy. To calculate magnetic energy, we set up a coordinate in the model of the chain of the ellipsoid-rings, as shown in Fig. 1(c). In this coordinate, a magnetic nanotube is put into the x-z plane with an angle θ_0 to z axis to display the angular dependence of the magnetic reversal processes; at the same time, the external field $\boldsymbol{H}$ is assumed to be applied along the z-axis. Considering the fanning rotation of magnetic moments, all the dipoles of ellipsoids in the same ring are assumed to congruously make an angle of α to the axis of the nanotubes and the dipoles in the neighbour rings make an angle of -α to the axis of the nanotubes, as shown in the inset of Fig. 1(c). For a chain of ellipsoid-rings model, there mainly exist three magnetic energies, i.e., exchange energy E_{ex}, Zeeman energy E_{ze} and anisotropy energy E_{an}.

The magnetostatic energy E_{ex} is described as the summation of dipole energy between all magnetic moments of the ellipsoids. According to our previous work (the details are included in the supplementary information), it can be calculated as

$$E_{ex}=\frac{N_r\mu_e^2}{2}\sum_{j=0}^{N_e-1}\sum_{i=1}^{N_e-1}\frac{1-3\left(1-\cos^2\alpha\right)\sin^2\left(\phi_j+\frac{\pi i}{N_e}\right)}{\left\{2\left(R-r_e\right)^2\left[1-\cos\left(2\pi i/N_e\right)\right]\right\}^{3/2}},\qquad(1)$$
$$+\frac{N_rN_eK_{N_r}\mu_e^2}{\left(2kr_e\right)^3}\begin{bmatrix}L_{N_r}\left(\cos2\alpha-3\cos^2\alpha\right)\\+M_{N_r}\left(1-3\cos^2\alpha\right)\end{bmatrix}$$

where,

$$L_{N_r}=\sum_{i=1}^{\frac{1}{2}(N_r-1)<i\le\frac{1}{2}(N_r+1)}\frac{N_r-(2i-1)}{N_r(2i-1)^3},$$

$$M_{N_r}=\sum_{i=1}^{\frac{1}{2}(N_r-2)<i\le\frac{1}{2}N_r}\frac{N_r-2i}{N_r(2i)^3},$$

$$K_{N_r}=M_{N_r}+L_{N_r}=\sum_{i=1}^{N_r}\frac{N_r-i}{N_ri^3}.$$

The Zeeman energy E_{ze} is the summation of interactions between the external field and all the magnetic dipole moments in ellipsoids. To simplify the calculation, the number of the ellipsoid-rings is assumed to be an even number due to the fanning rotation of magnetic dipoles between the neighboring rings. Thus, the Zeeman energy E_{ze} can be calculated as

$$E_{ze}=\frac{1}{2}N_rN_eH\mu_e\cos(\alpha+\theta_0)+\frac{1}{2}N_rN_eH\mu_e\cos(\alpha-\theta_0).\qquad(2)$$

The anisotropy energy E_{an} is described as the difference of directions dependence of magnetic interaction. As the length-diameter ratio of magnetic nanotubes or nanowires tends to an infinity, a shape anisotropy becomes a dominating anisotropy in the model of a chain of ellipsoid-rings. To simplify the numerical calculation, therefore, we only consider the shape anisotropy of the ellipsoid and neglect the magnetocrystalline anisotropy. Thus,

$$E_{an}=\frac{1}{2}N_rN_eI_s\mu_e\left(N_t-N_0\right)\left(1-\cos^2\alpha\right),\qquad(3)$$

where $\boldsymbol{I_s}$ is the saturation magnetization of magnetic nanotubes and N_t and N_o are the shape demagnetization factor of the ellipsoid along the major and minor axis, respectively.

2.3 Total magnetic energy E_t of nanotube

Based on above analysis of magnetic energy in a chain of ellipsoid-rings model with fanning rotation, the total magnetic energy E_t is the summation of E_{ex}, E_{ze} and E_{an}, which can be simplified as

$$\begin{aligned} E_t &= E_{ex} + E_{ze} + E_{an} \\ &= \frac{1}{2}\left[d\cos^2\alpha + eH\cos(\alpha+\theta_0) + f \right] + \\ &\frac{1}{2}\left[d\cos^2(-\alpha) + eH\cos(-\alpha+\theta_0) + f \right] \end{aligned} , \quad (4)$$

where the coefficients of d, e, f of the Eq.(4) are calculated as follows:

$$\begin{aligned} d = &\frac{N_r\mu_e^2}{2}\sum_{j=0}^{N_e-1}\sum_{i=1}^{N_e-1}\frac{3sin^2\left(\varphi_j+\frac{\pi i}{N_e}\right)}{\left\{2\left(R-r_e\right)^2\left[1-\cos\left(2\pi i/N_e\right)\right]\right\}^{3/2}} \\ &-\frac{N_rN_eK_{N_r}\mu_e^2L_{N_r}}{\left(2kr_e\right)^3}-\frac{3N_rN_eK_{N_r}\mu_e^2M_{N_r}}{\left(2kr_e\right)^3} \\ &+\frac{1}{2}N_rN_eI_s\mu_e\left(N_t-N_o\right) \end{aligned} ,$$

$$e = \frac{N_r}{2}N_e\mu_e$$, and

$$\begin{aligned} f = &\frac{N_r\mu_e^2}{2}\sum_{j=0}^{N_e-1}\sum_{i=1}^{N_e-1}\frac{1-3sin^2\left(\varphi_j+\frac{\pi i}{N_e}\right)}{\left\{2\left(R-r_e\right)^2\left[1-\cos\left(2\pi i/N_e\right)\right]\right\}^{3/2}} \\ &+\frac{N_rN_e\mu_e^2\left(M_{N_r}-L_{N_r}\right)}{\left(2kr_e\right)^3}+\frac{1}{2}N_rN_eI_s\mu_e\left(N_t-N_o\right) \end{aligned} .$$

It is noted that the total magnetic energy E_t of Eq. (4) includes two parts of magnetization reversal process of fanning rotation: one part of E_{tc} corresponds to the clockwise rotation with an angle α to the nanotube axis; the other part of E_{ta} corresponds to the counterclockwise rotation with an angle $-\alpha$ to the nanotube axis, as shown in the inset of Fig. 1(c). As the calculation of magnetic properties depends on the component of magnetic dipoles along the direction of applied field (i.e., z-axis) which is related to the angle between dipoles and z-axis, we set $\theta' = \alpha + \theta_0$ and $\theta'' = -\alpha + \theta_0$ to replace the α angle in Eq. (4) to demonstrate two angles of the dipoles intersect z-axis during fanning rotation. Thus, the total magnetic energy E_t can be rewritten as

$$\begin{aligned} E_t &= E_{tc} + E_{ta} \\ &= \frac{1}{2}\left[d\cos^2(\theta'-\theta_0) + eH\cos\theta' + f \right] \\ &+\frac{1}{2}\left[d\cos^2(\theta''-\theta_0) + eH\cos\theta'' + f \right] \end{aligned} . \quad (5)$$

Interestingly, the expression of total magnetic energy E_t in the Eq. (5) is very similar to that of S-W model in mathematical form, indicating the same underlying physics. Therefore, the model of chain of ellipsoid-rings with fanning rotation in magnetization reversal process can be used to simulate the magnetic properties of nanotubes.

3. Results and discussion

3.1 Magnetic hysteresis loop

To evaluate the magnetic behavior of nanotubes, we calculate the magnetic properties by simulating their hysteresis loops (i.e. *MH* curve), the curve of relative magnetization $\boldsymbol{I/I_s}$ versus applied field $\boldsymbol{H}$. In the model of chain of ellipsoid-rings with fanning rotation of magnetic moments, the relative magnetization of $\boldsymbol{I/I_s}$ is the sum of projection of clockwise dipoles and counterclockwise dipoles along z-axis, being equal to $\cos\theta'+\cos\theta''$ in mathematics. According to Fig. 1(c), the $\cos\theta'$ and $\cos\theta''$ can be figured out by calculating the equilibrium values of θ' and θ'' at various values of H, which can be obtained by setting $\partial E_{tc}/\partial\theta' + \partial E_{ta}/\partial\theta'' = 0$ (see Eq.(5)). Thus, the equation of magnetic hysteresis loop to be solved is changed into the following equation:

$$\begin{aligned} \frac{\partial E_{tc}}{\partial\theta'}+\frac{\partial E_{ta}}{\partial\theta''} &= \frac{1}{2}\left[-d\sin2(\theta'-\theta_0)-eH\sin\theta'\right] \\ &+\frac{1}{2}\left[-d\sin2(\theta''-\theta_0)-eH\sin\theta''\right]=0 \end{aligned} . \quad (6)$$

Figure 2 shows the angular θ_0 dependence of magnetic hystersis loops calculated from the Eq. (6). For simplicity, the value of $-2d/e$ is denoted as the abscissa. It is clearly seen that the magnetic properties of nanotubes are dependent on the value of θ_0; the magnetic hysteresis loops gradually change from the rectangle shape to the linear shape with θ_0 increasing from 0^o to 90^o, as shown in Fig. 2(a)-(e). This means that the magnetic properties of nanotubes are anisotropic, arriving at the maximum values (i.e., rectangle MH curve) when the nanotubes are put along the direction of applied field ***H***. Furthermore, all the magnetization of different θ_0 tend to the saturation value of I/I_s=1, while the applied field is increased large enough. It is interesting to note that the above results are similar to that calculated from S-W model. This is obviously due to the similar expression of total magnetic energy E_t between chain of ellipsoid-rings model and S-W model.

To well describe magnetization reversal process, we calculate two characteristic fields of magnetic hysteresis loops: one is the switching field H_s, where the magnetic moments reverse discontinuously; the other is the coercive field $\boldsymbol{H_c}$, where the net magnetic moments along the direction of ***H*** are zero. For the switching field $\boldsymbol{H_s}$, it is defined as $\partial H/\partial M$ =0 in the *MH* curve, which can be calculated by setting zero of the second order derivative of E_{tc} and E_{ta} in Eq. (5) with respectively respect to θ' and θ", namely,

$$\frac{\partial^2 E_{tc}}{\partial \theta'^2}+\frac{\partial^2 E_{ta}}{\partial \theta''^2}=[d\cos 2(\theta'-\theta_0)+eH\cos\theta'] +[d\cos 2(\theta''-\theta_0)+eH\cos\theta'']=0 \quad . \ (7)$$

Comparing Eq. (5) with Eq. (7), the H_s can be obtained by removing θ' and θ'', and becomes

$$H_s=-\frac{2d}{e}(\cos^{\frac{2}{3}}\theta_0+\sin^{\frac{2}{3}}\theta_0)^{-\frac{3}{2}} \quad . \quad (8)$$

For the coercive field H_c, it can be calculated by setting $\boldsymbol{I/I_s}$= cosθ'+cosθ'' =*0* in the Eq. (5) according to its mathematical definition, and thus the H_c becomes

$$H_c=\begin{cases}-\frac{2d}{e}(\cos^{\frac{2}{3}}\theta_0+\sin^{\frac{2}{3}}\theta_0)^{-\frac{3}{2}},(0°<\theta_0\le 45°)\\ -\frac{d}{e}\sin 2\theta_0,(45°<\theta_0\le 90°)\end{cases} \quad . \ (9)$$

Figure 2(f) shows the θ_0 dependence of switching field H_s and coercive field H_c. It is seen that when 0° <θ_0≤45°, H_s and H_c coincide with each other. This means that the magnetization switches abruptly at the field of H_c and the coercivity of nanotube is equal to H_s. But, when 45° <θ_0≤90°, H_c diverges from H_s and the magnetization switches abruptly at the field of H_s greater than H_c. Thus, the coercivity becomes less than H_s and then is reduced to zero at the angle θ_0 equal to 90°. This means that the magnetic nanotubes have the maximum coercivity while the applied field ***H*** is along the tube axis (i.e., θ_0=0°).

3.2 Geometrical parameter dependence of magnetic properties

To investigate the magnetic properties in a whole range of tubular geometry, the effects of geometrical parameters on the coercivity of nanotubes are discussed as follows. Such parameters include the number of rings (N_r) the axial ratio of an ellipsoid (*k*) and the wall thickness ratio ($\Delta R/R$) of nanotube.

Figure 3 demonstrates the dependence of coercivity on the number of rings N_r, and the axial ratio of an ellipsoid *k*. For a brief discussion, the value of θ_0 is set to be 60^o, and the wall thickness ratio $\Delta R/R$ is set to be 0.2. As shown in Fig. 3(a), the coercivity of nanotubes varies with the change of *k* and N_r values in the *k*-N_r space. It is seen that the shape of the ellipsoid greatly influences the magnetic properties of nanotubes. With the increase of the *k* value from zero, the coercivity decreases quickly and then increases to infinity, as shown in Fig. 3(b). Here, we define the k_{min} value as the minimum coercivity. It is interesting to note that such a k_{min} value changes with the increasing of N_r, and it will reach a fixed value of 0.98 when N_r is larger than 80. The k_{min}=0.98 is a critical value and therefore the coercivity is dramatically changed in the vicinity of k_{min}, as will be seen in the calculation of coercivity in the magnetic nanotubes of Fe, Co, Ni, Fe_3O_4 and $CoFe_2O_4$ (see Table 1). At the same time, we note that k_{min} value of 0.98 is close to an unity, where an ellipsoid becomes a sphere and its shape anisotropy disappears. Obviously, it is caused by the minimum of total magnetic energy and thus the magnetic nanotubes can stably exist in nature.

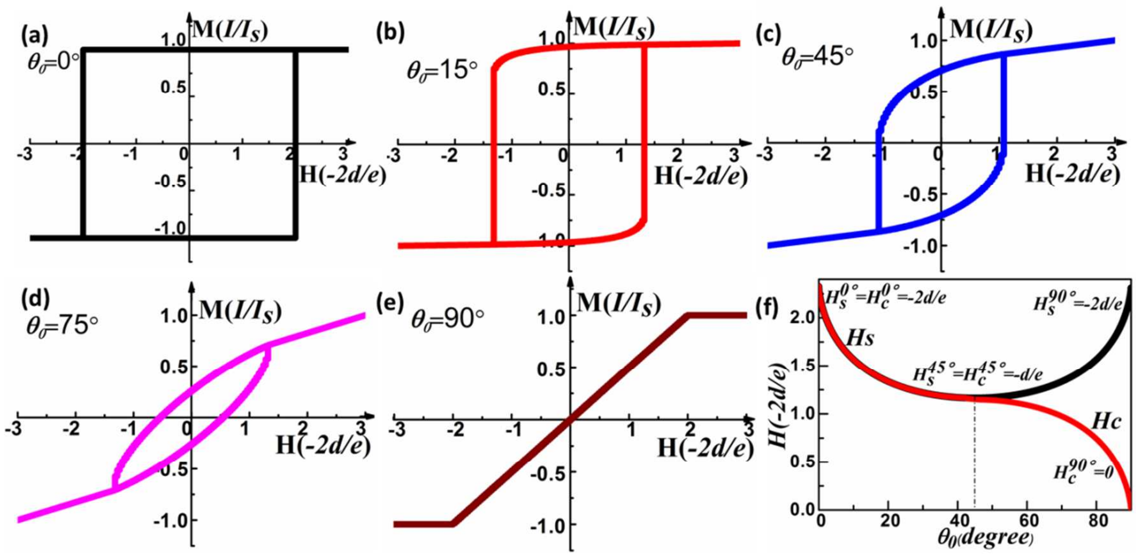

Fig.2 Angular θ_0 dependence of magnetic hysteresis loops calculated from Eq. (6). (a) $\theta_0=0^0$. (b) $\theta_0=15^0$. (c) $\theta_0=45^0$. (d) $\theta_0=75^0$. (e) $\theta_0=90^0$. (f) θ_0 dependence of switching field H_s and coercive field H_c.

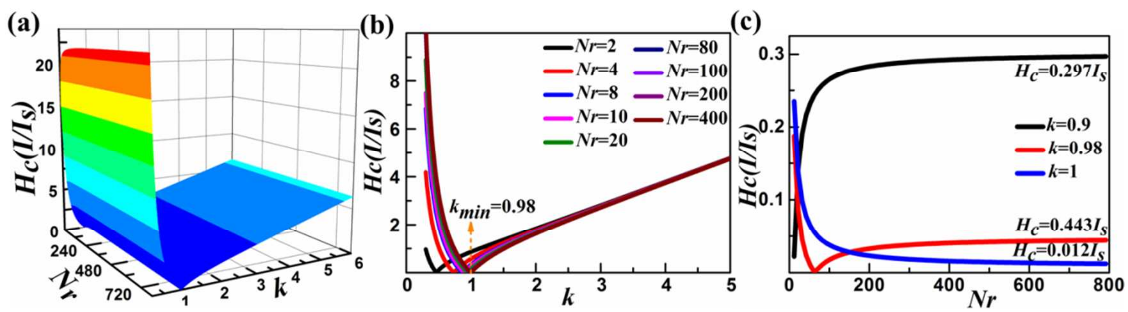

Fig.3: Influence of geometric parameters on the magnetic properties of nanotubes. (a) the coercivity of nanotubes varies with the change of k and N_r values in the k-N_r space; (b) k dependence of coercivity, $\boldsymbol{H_c}$, with different N_r; k_{min} is defined as a point in the $\boldsymbol{H_c}$-k curve to be corresponding to the minimum coercivity, and thus, when N_r is larger than 80, the k_{min} will attend to be a fixed value of 0.98. (c) N_r dependence of coercivity, $\boldsymbol{H_c}$, at the case of k=0.9, k=0.98 and k=1.

Thus, we choose three different k values around 0.98 to study the relationship between the coercivity $\boldsymbol{H_c}$ and the number of rings, Nr, as shown in Fig. 3(c). It is clearly seen that there exists dramatic changes of Nr to $\boldsymbol{H_c}$ with different k. When k is set to the critical value of 0.98, with the increase of Nr, the coercivity of nanotube decreases sharply to zero at first, and then increases slowly to a finite value of 0.443***Is***. When k value is less than 0.98 (i.e. k=0.9), the coercivity of nanotube increases quickly and then tends toward a finite value of 0.297 ***Is***; this is mainly due to the raid increase of shape anisotropy along the tube axis. But when k>0.98, the change in coercivity is the opposite: it decreases at the beginning and then rises up to reach a small but stable value (i.e. k=1), which is also due to the shape anisotropy.

Except the number of rings (N_r) and the axial ratio of an ellipsoid (k) there also exist another important parameter, the wall thickness of magnetic nanotubes (ΔR). Just due to the wall thickness, the magnetic nanotubes can be applied more widely than nanowires. Such a ΔR is limited within the critical size of a single-domain particle, because our model of chain of ellipsoid-rings is based on the single-domain particle.

To well depict the tube geometry, we use the parameter of wall thickness ratio ($\Delta R/R$) instead of wall thickness (ΔR) to discuss the change of coercivity. The values of $\Delta R/R$ are varied from 0 to 1 based on the experimental case [27-31]. Figure 4 demonstrates the influence of wall thickness $\Delta R/R$ on the coercivity $\boldsymbol{H_c}$ at the critical value of k=0.98 and N_r=400. It is seen that, with the increase of $\Delta R/R$, the coercivity of nanotube decreases at first to the minimum when the value of $\Delta R/R$=0.61 and then increases rapidly to the maximum when $\Delta R/R$=1; this is attributed to the change of shape anisotropy along the tube axis. Also, our model of chain of ellipsoid-rings can be used to calculate the magnetic properties of nanowire when the $\Delta R/R$ is close to 1. Thus, according to this model, we can predict that the nanowires shall possess the extreme value of coercivity, as shown in Fig. 4.

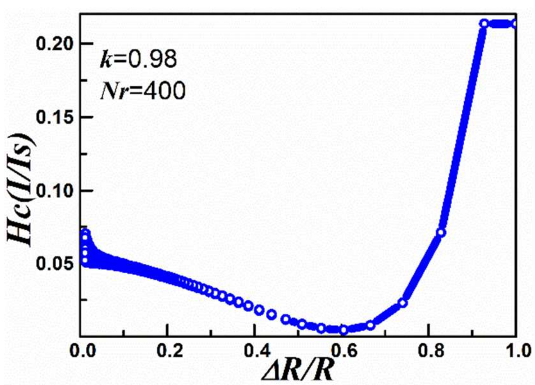

Fig. 4: Wall thickness ratio of nanotube, $\Delta R/R$, dependence of coercivity, $\boldsymbol{H_c}$, when the axial ratio of an ellipsoid, k, is 0.98.

3.3 Compare different rotation methods, different models, and the calculated values with experimental values

Based on the ellipsoid-ring model, we have used two mechanisms of magnetization reversal process (i.e., the fanning rotation and coherent rotation) to calculate the magnetic properties of nanotubes. The detailed calculation of coercivity in the fanning rotation and coherent rotation is included in the supplementary information. After making the comparisons to the influence of these two rotation processes on the magnetic properties of nanotubes, we can see that the angular θ_0 dependence of magnetic hysteresis loops of the two reversal mechanisms (as shown in Fig. 5) are similar, and the coercivity for fanning rotation is about half of that in the coherent rotation. Furthermore, compared with the Ref. 22 [24], the influences of the geometric parameters of the magnetic nanotubes on the coercivity $\boldsymbol{H_c}$ follow the same rules. For example, with increasing of the number of rings N_r, the $\boldsymbol{H_c}$ rises up at the beginning and then tends to a finite value when k is smaller than the limited k_{min}.

In addition, the S-W model is the classical and common model which is usually used to calculate the magnetic properties of nanotubes. From the Eq.(4), the total magnetic energy of chain of ellipsoid-rings model with fanning rotation seems different from the S-W model or the chain of ellipsoid-rings model with coherent rotation in mathematical equation. However, they are same in underlying physics with each other. In fanning reversal mechanism, there exist two kinds of rotated processes, i.e. clockwise rotation and counterclockwise rotation. Obviously, the total magnetic energy is the sum of these two kinds of reversal energy, E_{tc} and E_{ta}, as shown in Eq. (5). This means our model of chain of ellipsoid-rings is consistent with the S-W model in physics and thus can be used to calculate the magnetic properties of small particles.

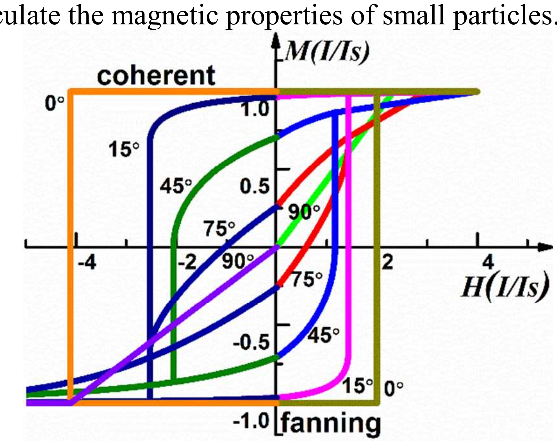

Fig.5: Angular θ_0 dependence of magnetic hysteresis loops using different rotation mechanisms.

Based on our ellipsoid-rings model with fanning rotation, we calculate coercivity of some common materials, such as Fe, Co, Ni, Fe_3O_4 and $CoFe_2O_4$ [27-31], and compare the calculated value of coercivity with the experimental value, then figure out the optimum k value, as shown in Table 1. The value of N_r is set as 400 according to Fig. 3(c) and the $\Delta R/R$ is determined according to their experimental data. As seen in Table 1, there exist the optimum k value for all the magnetic nanotubes, Fe, Co, Ni, Fe_3O_4 and $CoFe_2O_4$. It is

Table1: Comparison of calculated magnetic properties based on the model of ellipsoid-rings and experimental data found in the Fe, Co, Ni, Fe_3O_4 and $CoFe_2O_4$ nanotubes [27-31].

Magnetic nanotubes	*Is(G)*	*ΔR/R*	***Hc**(Oe)* Experimental results	***Hc**(Oe)*				Fanning	Coherent[24]
				k=0.8	*k*=0.98	*k*=1	*k*=1.2	*k* (optimum)	*k* (optimum)
Fe	1729	0.1667	110	2352.11	123.43	69.83	1663.44	0.985	/
Co	1430	0.26	200	1925.20	84.26	84.89	1405.63	0.963	1.06
Ni	485	0.49	610	633.46	52.51	52.27	505.46	0.806	1.24
Fe_3O_4	715	0.14	850	975.16	26.18	26.01	685.01	0.816	1.08
$CoFe_2O_4$	193	0.6	136	250.33	23.09	84.95	203.66	0.872	/

interesting to note that all the optimum *k* values of above magnetic nanotubes with fanning rotation are less than unity; but the optimum *k* values greater than unity in the coherent rotation, as shown in the last column of Table 1. This suggests that the magnetic nanotubes with chain of oblate-ellipsoid rings prefer to the fanning rotation, on the contrary, the magnetic nanotubes with chain of prolate-ellipsoid rings prefer to the coherent rotation. This interesting prediction waits further experiments to verify. Consequently, a chain of ellipsoid-rings model with both fanning and coherent rotation can be used to calculate the magnetic properties of nanotubes.

5. Conclusion

In this article, we investigate the fanning reversal mechanism of the magnetic nanotube in the chain of ellipsoid-rings model, and calculate the magnetic properties of nanotubes, including switching field $\boldsymbol{H_s}$ and coercibity field $\boldsymbol{H_c}$, and then systematically discuss the influence of geometric parameters, the number of rings N_r, the axial ratio of single ellipsoid k and the wall thickness of nanotube $\Delta R/R$, on the magnetic properties of nanotubes. The conclusions are as follows: (1) There exist a *k* value to correspond to the minimum coercivity. When N_r is more than 80, such a *k* value tends to the fixed value of 0.98. Thus, in order to enhance the coercivity, we can control the *k* far away from 0.98 in the experiment. (2) When the number of rings N_r is larger than 400, the coercivity of magnetic nanotube tends to be a finite value, and different *k* has different value. (3) With the increasing of wall thickness $\Delta R/R$ of nanotube, the coercivity $\boldsymbol{H_c}$ will decrease firstly and then increase sharply to the maximum value when $\Delta R/R$=1 at *k*=0.98. In this case, the nanotube will be the nanowire. (4) Our model of chain of ellipsoid-rings with fanning reversal mechanism can be used to calculate small particles, especially for the nanotubes and nanowires. (5) It is interesting to predict that the magnetic nanobutes with chain of oblate-ellipsoid rings prefer to fanning rotation, on the contrary, the magnetic nanotubes with chain of prolate-ellipsoid rings prefer to coherent rotation.

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