Monte Carlo simulation study on magnetic hysteresis loop of Co nanowires

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Abstract; The influence of temperature on the magnetic hysteresis and coercivity of Co magnetic nanowires was investigated by Monte Carlo method. Monte Carlo simulation results of hysteresis loop indicated that both its tendency and the coercivity were consistent with experimental results within a given error. The coercivity was calculated with the temperature and the angle between nanowires and magnetic field applied, varying the temperature from 50K to 300K for Co nanowires with a diameter of 30nm. The coercivity decreased monotonically at all values of angle with the increase of temperature T, following the parabolic curve of T^{γ} . The power exponent γ , determined corresponding to angle between nanowires and magnetic field, was $0.03\sim0.06$ and was consistent with the previous experimental results.

Keywords;Monte Carlo method, nanowire, coercivity, magnetic hysteresis loop **Corresponding author;** yongsonhong77@yahoo.com

1. Introduction

Because of huge potential application of Co nanowires in ultrahigh density perpendicular magnetic recording field, their magnetic properties were widely investigated and the magnetic hysteresis loops were determined experimentally in recent years [1-9].

MC (Monte Carlo) simulation of magnetic hysteresis loops of magnetic nanowires at room temperature was performed and the accuracy of simulation was identified in comparison with experimental results in [1-3]. Because the simulation environment was taken at room temperature, the influence of temperature on the coercivity could not be regarded. In this work, based on the MC method, the magnetic hysteresis property of Co nanowires was investigated.

2. Modeling and method

Monte Carlo simulation was conducted for the Co nanowires with a diameter of 30*nm* and a length of 600*nm* and investigated experimentally and fully so as to identify the accuracy of simulation method.

Assuming nanowire is a finite cylinder of which the aspect ratio is 20, this cylinder can be divided by small regular global-shaped cells which have their spin.

Considering the exchange interaction energy, the dipolar interaction energy, the anisotropy energy, and Zeeman energy for this model, the total energy of the system can be written as follows.

$$E = -\sum_{ij} J \vec{S}_{i} \cdot \vec{S}_{j} + D \sum_{i < j} \left[\frac{\vec{S}_{i} \cdot \vec{S}_{j}}{r_{ij}^{3}} - \frac{\vec{S}_{i} \vec{r}_{ij} \cdot \vec{S}_{j} \vec{r}_{ij}}{r_{ij}^{5}} \right] - K \nu_{0} \sum_{i} \left(\vec{S}_{i} \cdot \vec{\mu}_{i} \right)^{2} - M_{s} \nu_{0} H \sum_{i} \vec{S}_{i} \cdot \vec{h}$$
(1)

The first term is the exchange interaction energy, where $J=2Ad\pi/6$; d is the diameter of the unit cell, A is the exchange of coupling between unit cells, and \vec{S}_i is the spin of the i^{th} unit cell.

The second term is the dipolar interaction energy, where $D = (M_S v_0)^2 / 2$ (*Ms* is saturation magnetization) denotes the strength of the dipole-dipole interaction; $v_0 (= \pi d^3 / 6)$ is the volume of the cell; r_{ij} is the vector for the displacement between sites *i* and *j*.

The third term represents the magnetocrystalline anisotropy energy, where K is the magnetic anisotropy constant, $\vec{\mu}_i$ is the unit vector of easy axis.

The last term represents Zeeman energy, where *H* is the magnetic field applied and \vec{h} is the unit vector of applied field.

The typical material parameters used in this work are $A = 1.3 \times 10^{-11} J/m$, $M_s = 1.43 \times 10^6 A/m$, $K = 4.5 \times 10^5 J/m^3$. The temperature was varied between 50K and 300K and the free boundary condition was used for both directions of the length and the diameter such that the feature of nanowires appears. And the metropolis algorithm was used in the simulation of the reversal process of spin.

3. Results and discussion

Figure 1 shows the magnetic hysteresis loops at 300K with an angle H_{α} between nanowires and magnetic field. It is found that MC simulation result of magnetic hysteresis loops is consistent with experimental result in both tendency

and coercivity H_c .

Considering the effect of magnetocrystalline anisotropy, the coercivity decreases with the increase of angle H_{α} and is not zero at 90° and therefore this is consistent with general hysteresis property. However, the coercivity is approximately zero in the absence of the magnetocrystalline anisotropy (that is, K=0). This shows that the angle between the applied field and nanowire as well as magnetic anisotropy is important factor on coercivity.

According to previous study, if the nanowires are infinite lengthy cylinders and the magnetocrystalline anisotropy is much less than the shape anisotropy, it was reported that the rectangular magnetic hysteresis loops were obtained in external magnetic field applied along the axis. However, in case of Co, the magnetocrystalline anisotropy constant is $K=4.5\times10^5$ J/m³ and is almost equal to that of shape anisotropy. That is, the simulation result identifies that it is not negligible.



Fig 1. Hysteresis loops of Co nanowires at various angles (M-magnetization intensity, M_s-saturation magnetization)

Figure 2 gives the results of the coercivity calculated with temperature and angle H_a , for Co nanowires with a diameter of 30*nm*, varying the temperature from



Fig. 2. Variation of the coercivity with temperature and angle



Fig. 3. Angular dependence on the variation of the coercivity of Co nanowires at 300K with various diameters (30*nm*, 40*nm*, 70*nm*)

As the figure shows, the coercivity decreased monotonically at all values of H_{α} , with the increase of temperature, following the parabola of the $T^{-\gamma}$ shape. The power exponent γ , determined corresponding to H_{α} , was 0.03~0.06 and was consistent with the previous experimental results [10].

Figure 3 shows the variation of the coercivity of nanowires with thickness and angle H_{α}

The magnetic reversal process was investigated to consider the mechanism of magnetic reversal of Co nanowires. Figure 4 shows the state of the magnetic reversal of Co nanowires with a diameter of 30nm at $H_{\alpha} = 0^{\circ}$ as the time goes.

Fig. 4. Spin reversal process with time at $H_{\alpha}=0^{\circ}$ in a magnetic field of -318kA/m

The simulation shows the reversal nucleus is formed from both sides and propagates in case of small angle H_{α} for the nanowires with small diameter. That is, the magnetic reversal propagates with localized nucleation.

The reversal nucleus is formed at both sides of nanowires around the magnetic field where it takes place (Fig 4.a) and is propagated (Fig 4.b) and the reversal

process is completed (Fig 4.c-d). What is important here is the fact that the other spins remain constant when the nucleus is formed and propagated.

However, in case of angles greater than 80°, that is, at $H_{\alpha} = 90^{\circ}$, the spin considered is turned round to the direction of magnetic field applied without the nucleation at both sides and this can be explained by the coherent reversal model and is consistent with the result obtained from the relationship between coercivity and angle.

In the simulation of magnetic reversal process in Co nanowires with a diameter of 95*nm* with the increase of magnetic field, it is found that all the spins are not reversed at the same time but rotated in and they reverse with the increase of diameter in the form of curling reversal unlike nanowires with small diameter.

Conclusions

In conclusion, the mechanism of nanowires is fairly complicated and it is associated with the diameter of nanowires and the direction of external magnetic field. But the defect of surface structure present in nanowires will be influential in the magnetic reversal process of nanowires.

References

- R.Skomski, H.Zeng, and D.J.Sellmyer, Incoherent magnetization reversal in nanowires, J. Magn. Magn. Mater. 249 (2002) 175–180
- [2] C.Verdes., et.al, J. Magn. Magn. Mater. 304 (2006), 27-31
- [3] W.Z.Zhang, W.Guo, L.Wang, K.H. Höglund, A.W. Sandvik, Effects of ed ge disorder in nanoscale antiferromagnetic clusters, Phys. Rev. B 82, 0124 01
- [4] R.Skomski, H.zeng, D.J.Sellmyer, Magnetic localization in transition-metal nanowires, Phys Rev. B62 (2000), 3900-3904
- [5] L.C.Sampaio, E.H.C.P.Sinnecker, G.R.C.Cernicchiaro, M.Knobel, M.Vazquez, J.Velazquez, Magnetic microwires as macrospins in a long-range dipole-dipole interaction, Phys Rev. B61 (2000), 8976-8983
- [6] P.M.Paulus, F.Luis, M.Kroll, G.Schmid, Low-temperature study of the magnetization reversal and magnetic anisotropy of Fe, Ni, and Co nanowires, J.

Magn. Magn. Mater. 224 (2001), 180-196

- [7] X.Y.Zhang, G.H.Wang, T.F.Chan, P.K.Zheng, X.X.Zhang, N.Wang, Fabrication and magnetic properties of ultrathin Fe nanowire arrays, Appl. Phys. Lett.83 (2003), 3341-3343
- [8] Abdolali Ramazani, Mohammad Almasi Kashi, Ghafour seyedi, Crystallinity and magnetic properties of electodeposited Co nanowires in porous alumina, J. Magn. Magn. Mater. 324 (2012), 1826-1831
- [9] R.Lavin, C.Gallardo, J.L.Palma, J.Escrig, J.C.Denardin, Angular dependence of the coercivity and remanence of ordered arrays of Co nanowires, J. Magn. Magn. Mater. 324 (2006), 2360-2362
- [10] Naeem Ahmad, J. Y. Chen, Javed Iqbal, W. X. Wang, W. P. Zhou et al., Temperature dependent magnetic properties of Co nanowires and nanotubes prepared by electrodeposition method, J. Appl. Phys. 109(2013), 07A331