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ORIGINAL PAPER

Antiferromagnetic properties of *CoO* nanoparticle: a Monte Carlo simulation

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Abstract: The magnetic properties of antiferromagnetic *CoO* compound have been studied using Monte Carlo simulations within the Ising model framework. The thermal magnetizations and magnetic susceptibilities are computed for a fixed size. In addition, the Néel temperature is deduced. The magnetization versus the reduced exchange interactions and crystal field are studied for a fixed system size, $N = 10$ nm particles. The magnetic hysteresis cycle versus temperature is also established.

Keywords: Compounds; Monte Carlo simulations; Néel temperature; Magnetic hysteresis; Reduced exchange interactions; Coercive field

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1. Introduction

Bulk *CoO* is known to be an insulating antiferromagnet with rocksalt cubic structure and Néel temperature of 298 K [1]. In 1961, Néel suggested that small antiferromagnetic nanoparticles (AFN) should exhibit superparamagnetism or weak ferromagnetism [2]. He attributed the permanent magnetic moment to an uncompensated number of spins on two sublattices. Naturally, the magnetic behavior of cubic *CoO* nanoparticles has been widely studied in the next half a century [3–6]. The magnetic properties of *CoO* nanoparticles have been studied by many authors [7–10]. New challenging questions are posed by the observation of exchange bias on nanoparticle systems, when one phase is ferromagnetic (FM) and the other one is spin glass (SG) [11–14], playing the role of the antiferromagnet (AF) in pinning the FM magnetization so as to minimize the interface exchange interaction energy. The net magnetization of *CoO* is assumed to be mainly due to uncompensated spins within the AF particles or at their interfaces [15]. The latter naturally explains why exchange bias in metal oxides and other binary transition metal compounds does not systematically depend on crystalline interface orientation [13]. The magnetic properties of ferromagnetic *ErC* compound have been studied using the Monte Carlo simulation [16]. In this work, we are interested in the magnetic properties of *CoO* compound. The thermal magnetizations and magnetic susceptibilities have been computed for a fixed size. The Néel temperature has been deduced. The magnetization versus the reduced exchange interactions and crystal field have been studied for a fixed system size, $N = 10$ nm particles and a fixed temperature. The magnetic hysteresis cycle with temperature has been also established.

2. Theoretical methods

We consider a antiferromagnetic *CoO* nanoparticle with cubic structure as shown in Fig. 1. The Hamiltonian of the

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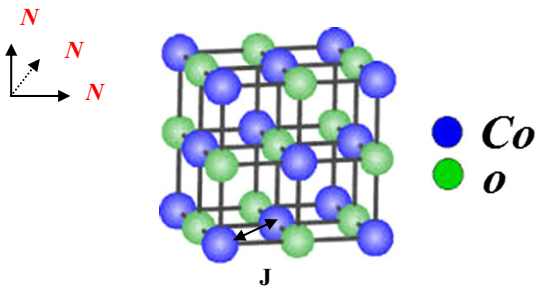

Fig. 1 *CoO* cubic structure

Ising model includes nearest neighbor interactions and external magnetic field:

$$H = -J\sum_{\langle i,j\rangle} S_i S_j - h\sum_i S_i - \Delta\sum_i S_i^2 \qquad (1)$$

where $\langle i,j\rangle$ stand for the first nearest neighbor sites i and j, corresponding to the coupling constants J. The external magnetic field h is applied over all the particles of the lattice structure in the z-direction and Δ is the crystal field. The magnetic spin moments $S_i = 3/2$. The reduced exchange interaction, $J = -11$ K, has been deduced from $J = \frac{\theta_{CW}(K)}{30}$ given by mean field theory, where the Curie–Weiss temperature is $\theta_{CW}(K) \approx -330$ K [17]. The spins point along (001) [18, 19]. The anisotropy field acting on the *Co* ions is mostly single-ion anisotropy (orbital effect, etc.) and is much larger than that of the *O* ion that originates mainly from magnetic dipole interactions [20]. In this work, the magnetization, magnetic susceptibility, magnetic field and crystal filed are unitless.

3. Monte Carlo simulations

In this work, we have considered the alternating AFM *Co* planes. The *CoO* compound is assumed to reside in the unit cells, and the system consists of the total number of particles $N \times N \times N$ with $N = 10$ nm particles. We apply a standard sampling method to simulate the Hamiltonian given by Eq. (1) with free boundary conditions on the lattice. The configurations have been generated by sequentially traversing the lattice and making single-spin flip attempts. The flips are accepted or rejected according to a heat-bath algorithm under the Metropolis algorithm. Our data have generated with 10^5 Monte Carlo steps per particle. The computer program discards the first 10^4 Monte Carlo simulations. In order to perform the numerical results, each Monte Carlo simulation starts from a different initial condition. Hence, we have performed the average of each parameter and estimated the Monte Carlo simulations, averaging over many initial conditions.

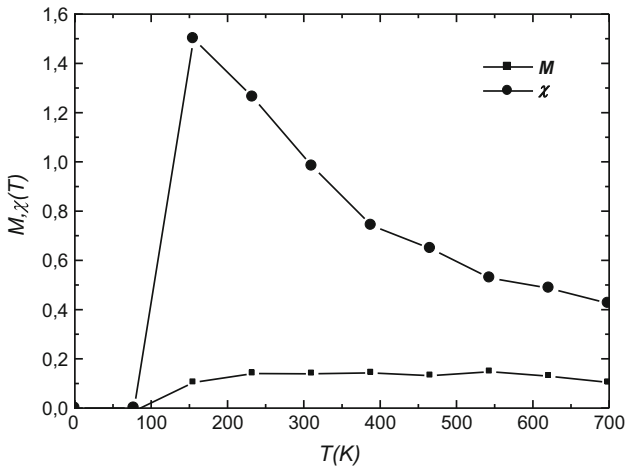

Fig. 2 Magnetization and magnetic susceptibility versus the temperature of *CoO* compound for $h = 0$ and $\Delta = 0$ with $N = 10$ nm particles

Our program calculates the following parameters, namely

The magnetizations per *Co* ion: $M = \left\langle \frac{1}{NNN}\sum_i \sigma_i \right\rangle$

$$= \frac{1}{NNN}\sum_i \langle\sigma_i\rangle = \frac{1}{NNN}\frac{\sum_i \sigma_i e^{-\beta E}}{\sum_i e^{-\beta E}} \qquad (2)$$

and E is the internal energy per *Co* ion:

$$E = \frac{1}{NNN}\langle H\rangle \qquad (3)$$

with

$$E = \frac{1}{NNN}\left\langle -J\sum_{\langle i,j\rangle}\sigma_i\sigma_j - h\sum_i \sigma_i - \Delta\sum_i \sigma_i^2 \right\rangle \qquad (4)$$

and the corresponding magnetic susceptibility is given by:

$$\chi = \frac{\beta}{(NNN)^2}\left(\left\langle\sum_i \sigma_i^2\right\rangle - \left\langle\sum_i \sigma_i\right\rangle^2\right) \qquad (5)$$

where $\beta = 1/k_B T$ and k_B is the Boltzmann's constant and the T denotes the absolute temperature.

4. Results and discussion

Figure 2 shows the variation of the magnetization and magnetic susceptibility versus the temperature of *CoO* compound for $h = 0$ and $\Delta = 0$ with $N = 10$ nm particles, for the reduced exchange interactions $J = -11.11$ K. The Néel temperature obtained is 155 K. This value is comparable with those reported earlier [21]. The variation of Néel temperature in ultrathin layers of *CoO* nanograins is low [21]. The saturation magnetization is 3/2. The

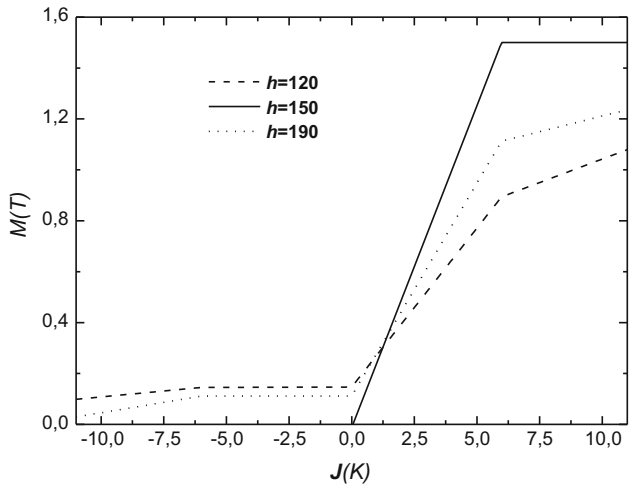

Fig. 3 Magnetization versus the reduced exchange interaction of *CoO* compound for $h = 120$, 150, 190 and $\Delta = 0$ with $N = 10$ nm particles and the temperature $T = 199$ K

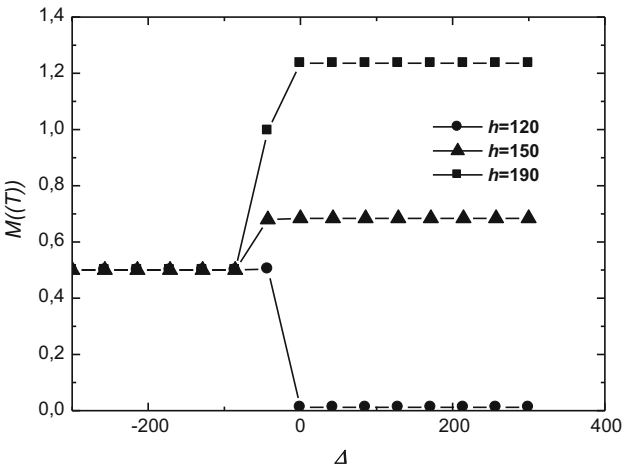

Fig. 4 Magnetization versus the crystal field of *CoO* compound for $h = 120$, 150 and 190 and $\Delta = 0$ with $N = 10$ nm particles and the temperature $T = 1$ K

dependence of the magnetization on the reduced exchange interaction, J, for a fixed size ($N = 10$ nm particles) and for two temperatures $T = 9$ and 99 K and external magnetic field ($h = 0$) and $\Delta = 0$ is shown in Fig. 3. The magnetization increases with the increase of the reduced exchange interaction for an external field for $h = 120$, 150 and 190. The behavior antiferromagnetic coupling, J, between Co^{2+} and Co^{2+} ions is shown in Fig. 4. It is found that the magnetization of the *CoO* is not affected by the antiferromagnetic negative J coupling values. When the coupling constant J undergoes positive values, the magnetization shows an abrupt change until it reaches the 1.25 value and remains constant. This behavior is observed in antiferromagnetic systems for an external field for $h = 120$, 150 and 190 and for $T = 1$ K. The magnetization versus the magnetic field (h) for $N = 10$ nm particles is presented in Fig. 5, for fixed values of temperature $T = 9$ and 99 K and a fixed value of the reduced exchange interactions $J = -11$ K.

From Fig. 5, it is observed that the coercive magnetic field h_C and remanent magnetization are equal to zero in *CoO* nanoparticle; consequently, this behavior is superparamagnetic. This behavior is comparable with those reported earlier [22, 23]. Both h_C and M_r are expected to decrease with increasing temperature. It is obtained that h_C decreases, while M_r increases. Considering the M_C simulations discussed above, the experimental behavior may thus be attributed to mixed interactions, an appreciable part of which being antiferromagnetic. This behavior has been observed in previous work [24]. *CoO* becomes superparamagnetic [25–27] for temperature $T = 5$ K.

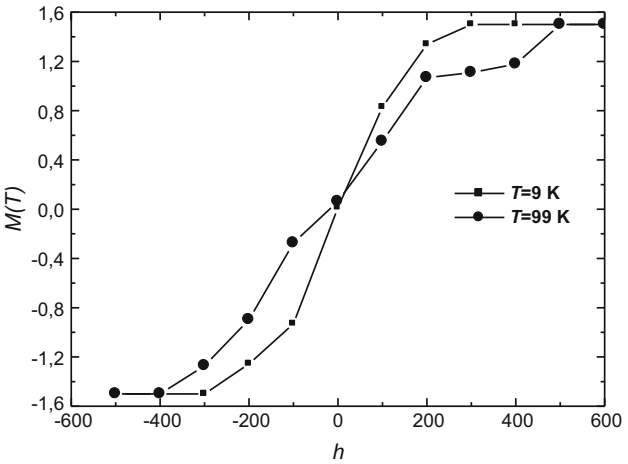

Fig. 5 Magnetic hysteresis cycle of *CoO* compound for the temperature $T = 9$ and 99 K for $N = 10$ nm particles

5. Conclusions

The Néel temperature is estimated for a zero external magnetic and zero crystal fields with $N = 10$ nm particles. The obtained value is sensitive with the increase in number of nanoparticles. The magnetization versus the reduced exchange interactions is deduced for fixed values of the temperature, zero external magnetic and crystal fields and $N = 10$ nm particles. The magnetic hysteresis cycle is deduced for a system $N = 10$ nm particles and for different temperature values. The remnant magnetization, saturation magnetization and magnetic field coercive are deduced for *CoO* nanoparticle.

References

[1] C N R Rao and B Raveau *Transition Metal Oxides* (New York: Wiley VCH) p 338 (1995)
[2] L Néel *Compt. Rend*. **252** 4075 (1961)
[3] L Y Zhang, D S Xue and C X Gao *J. Magn. Magn. Mater*. **267** 111 (2003)
[4] M Ghosh, E V Sampathkumaran and C N R Rao *Chem. Mater*. **17** 2348 (2005)
[5] D P Dutta, G Sharma, P K Manna, A K Tyagi and S M Yusuf *Nanotechnology*. **19** 245609 (2008)
[6] Z P Chen, A Q Xu, Y Zhang and N Gu *Curr. Appl. Phys.* **10** 967 (2010)
[7] J S Yin and Z L Wang *Phys. Rev. Lett.* **79** 2570 (1997)
[8] C F J Flipse, C B Rouwelaar and F M F de Groot *Eur. Phys. J. D*. **9** 479 (1999)
[9] L Soriano, M Abbate, A Fernandez, A R Gonzales- Elipe, F Sirotte and J M Sanz *J. Phys. Chem. B*. **103** 6676 (1999)
[10] M Verelst et al. *Chem. Mater*. **11** 2702 (1999)
[11] D Fiorani, A M Testa, E Bonetti, L Savini, and S Signoretti *Phys. Rev. B* **66** 174418 (2002)
[12] J Nogués et al. *Phys. Reports*. **422** 65 (2005)
[13] J Nogués and I K Schuller *J. Magn. Magn. Mater.* **192** 203 (1999)
[14] P K Manna and S M Yusuf *Phys. Reports.* **535** 61 (2014)
[15] M Gruyters *J. Magn. Magn. Mater*. **320** 407 (2008)
[16] R Masrour, L Bahmad, E K Hlil, M Hamedoun and A Benyoussef *Indian J. Phys*. **89** 699 (2015)
[17] C Kittel, *Introduction to Solid State Physics* (New York: Wiley) p 608 (1976)
[18] M D Rechtin and D L Averbach *Phys. Rev. B* **6** 4294 (1972)
[19] T J Moran and I K Schuller *J. Appl. Phys*. **79** 15 (1996)
[20] G Geis, R Geick, C R Becker, V Wagner *Physica B/*C. **86** 1257 (1977)
[21] M Molina-Ruiz, A F Lopeandia, F Pi, D Givord, O Bourgeois and J Rodrıguez-Viejo *Phys. Rev. B* **83** 140407(R) (2011)
[22] M Gruyters *Phys. Rev. Lett*. **95** 077204 (2005)
[23] M Gruyters *Europhys Lett*. **77** 57006 (2007)
[24] D Srikala, V N Singh, B R Mehta and S Patnaik *J. Magn. Magn. Mater*. **324** 2512 (2012)
[25] H Shi and X He. *J. Phys. Chem. Solids.* 73 646 (2012)
[26] T Ambrose and C L Chien. *Phys. Rev. Lett*. **76** 1743 (996)
[27] S Kundu, M D Mukadam, S M Yusuf and M Jayachandran *Cryst. Eng. Comm*. **15** 482 (2013)