



Revista Mexicana de Física

ISSN: 0035-001X

rmf@ciencias.unam.mx

Sociedad Mexicana de Física A.C.

México

Salazar-Enríquez, C.D.; Agudelo, J.D.; Restrepo, J.; Restrepo-Parra, E.
Monte Carlo study of the magnetic properties and finite size effects in single wall ferromagnetic
nanotubes

Revista Mexicana de Física, vol. 58, núm. 2, diciembre, 2012, pp. 123-126

Sociedad Mexicana de Física A.C.

Distrito Federal, México

Available in: <http://www.redalyc.org/articulo.oa?id=57030392031>

- [How to cite](#)
- [Complete issue](#)
- [More information about this article](#)
- [Journal's homepage in redalyc.org](#)

redalyc.org

Scientific Information System

Network of Scientific Journals from Latin America, the Caribbean, Spain and Portugal

Non-profit academic project, developed under the open access initiative

Monte Carlo study of the magnetic properties and finite size effects in single wall ferromagnetic nanotubes

C.D. Salazar-Enrriquez^{a,b}, J.D. Agudelo^{a,b,d}, J. Restrepo^c, and E. Restrepo-Parra^{a,b}
^aLaboratorio de Física del Plasma, Universidad Nacional de Colombia-Sede Manizales,
 A.A. 127 Manizales, Colombia.
 e-mail: cdsalazare@gmail.com
^bPCM Computational Applications, Universidad Nacional de Colombia-Sede Manizales,
 A.A. 127 Manizales, Colombia.
^cGrupo de Magnetismo y Simulación, Instituto de Física, Universidad de Antioquía,
 A.A. 1226 Medellín, Colombia.
^dUniversidad de Manizales, Facultad de Ingeniería,
 AA 127 Manizales, Colombia.

Recibido el 25 de junio de 2010; aceptado el 19 de enero de 2011

In this work the influence of diameter upon the magnetic properties of single wall ferromagnetic nanotubes was studied. Magnetization per site, magnetic susceptibility, specific heat and total energy were computed on the basis of a classical Heisenberg model involving nearest neighbor interactions and using a Monte Carlo method implemented with a single spin movement Metropolis dynamics. The spontaneous magnetization, absolute value of ferromagnetic energy and critical temperature increase with diameter of the tubes and spin quantum number. The critical temperature is determined by the tube diameter. As the diameter of the tube tends to infinity, all the numerical results approach to those of a two-dimensional monolayer.

Keywords: Nanotubes; magnetism; Monte Carlo.

En este trabajo se estudió la influencia del diámetro sobre las propiedades magnéticas de nanotubos ferromagnéticos de una sola capa. Se calcularon la magnetización por sitio, la susceptibilidad magnética, el calor específico y la energía total partiendo de un modelo clásico de Heisenberg y teniendo en cuenta interacciones de primeros vecinos, además se empleó el método de Monte Carlo con la dinámica de Metrópolis de movimiento de espín unitario. La magnetización espontánea, el valor absoluto de la energía ferromagnética y la temperatura crítica incrementan con el diámetro de los nanotubos y el número cuántico de espín. A medida que el diámetro de los nanotubos tiende a infinito, todos los resultados numéricos tienden a los de una capa bidimensional.

Descriptores: Nanotubos; magnetismo; Monte Carlo.

PACS: 75.25.-j; 75.30.Et; 75.70.-I; 75.75.-c

1. Introduction

Since the work published by Iijima about carbon nanotubes in 1991 [1], much attention has been paid on low dimensional structures such as nanodots, nanowires, nanoparticles and nanotubes. In particular, considerable efforts have been made in fabricating magnetic nanotubes due to their potential applications, such as ultrahigh-density magnetic storage devices, biotechnology, nanomedicine and electronic devices, among others [2-4]. Experimental works have reported successfully methods to fabricate ferromagnetic (FM) nanotubes, and their magnetic properties have been investigated [5-7]. The new experimental works which have been done recently in this area opened the way for the creation of nanotubes based on the composite molecules that contain metal atoms [8,9]. In this case, the nanotube is considered as a tube, composed of rectangular (square, or others) unit cells with spins situated in the vertices of the unit cells [10]. There are different theoretical methods for the investigation of magnetic nanotubes, such as micromagnetic simulation [11-13], continuum theory of ferromagnetism [14-17], and Monte Carlo simulations [10].

In this work, Monte Carlo simulations of magnetic properties in magnetic nanotubes based on the geometrically simple lattice with the square unit cell are present. The aim of this study is to found the dependence of the magnetic properties on the diameter (m = number of atoms per cross section), when the system presents values of anisotropy and exchange parameter in the same order of magnitude. Results seem to be similar to more realistic cases of magnetic nanotubes, *e.g.*, similar to those considered in the literature [8,9].

2. The model description

A classical Heisenberg model involving nearest neighbor interactions and Monte Carlo method implemented with single spin movement Metropolis dynamics was used. The Hamiltonian that describes the system (Eq. 1) contains a term regarding to exchange energy and other corresponding to the magneto-crystalline anisotropy.

$$H = -j \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j - K \sum_i (\vec{S}_i \cdot \hat{n}_i)^2 \quad (1)$$

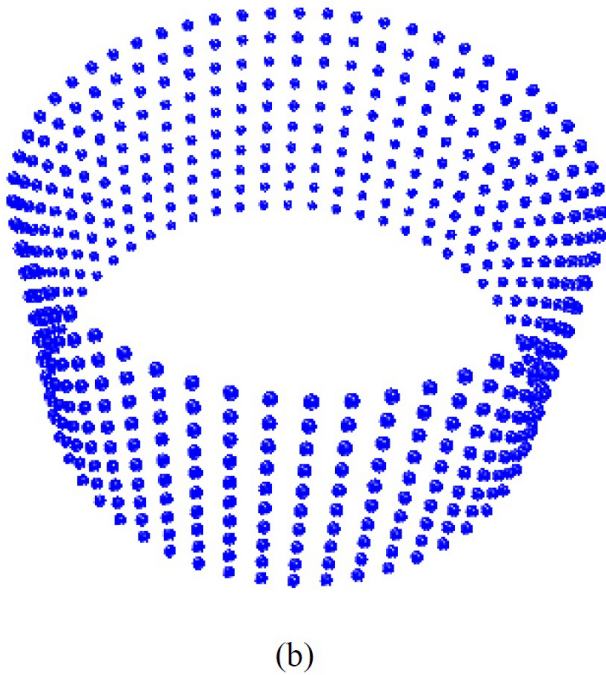
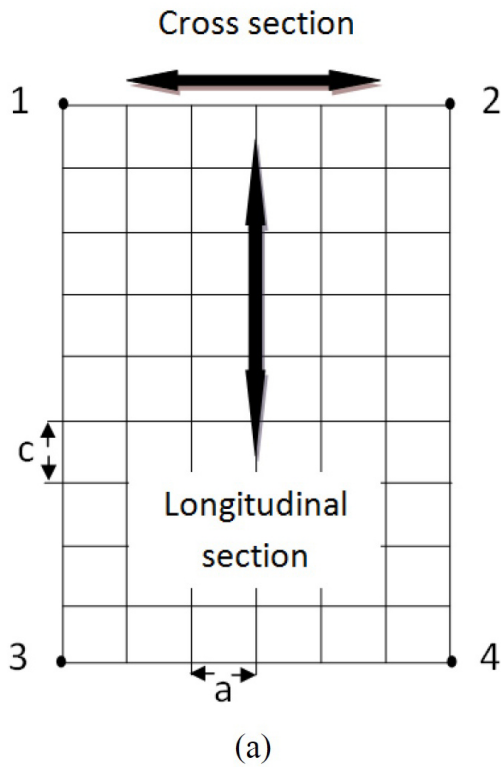


FIGURE 1. (a) 2D- monolayer arrangement of atoms. Each intersection is a magnetic site. For building the tube, a sheet of ions was rolled up linking the point 1 with the point 2 and the point 3 with the point 4 and (b) final scheme of the nanotube.

J is the exchange parameter, \vec{S}_i and \vec{S}_j are the spins, K is the anisotropy constant and \hat{n}_i is the easy axis direction. Atoms were arranged forming a rolled up simple square lat-

tice by keeping constant the lattice parameter of the sheet (c) (Fig. 1(a) and 1(b)). However, as the nanotubes curvature increases, the nearest distance between lattice sites in the cross section (a) decreases as well as the exchange parameter rises. The nearest distance between lattice sites (c) in the longitudinal section is kept constant. The nanotube diameter, denoted by m , is worked out by means of the number of magnetic ions in the cross section of the nanotube. In these calculations, numerical values were given for the exchange parameter of the sheet $J_s = 15$ meV, $K = 5$ meV, (longitudinal direction) and different quantum spin number (S) $S=1/2$, 1 and $3/2$. An exchange parameter depending on the cross section of nanotube (J_t) was proposed by Eq. 2, taking into account previous results reported [18]. The exchange parameter J_t comes from the J_s that is the exchange parameter of an atoms sheet. It seems natural because the physical properties of a nanotube tend to be similar to those of sheet as the diameter tends to infinity. The idea in this work is to evaluate as a first approximation the magnetic properties of the nanotubes, considering the contribution of the nearest neighbors to the magnetic coupling. It can be concluded that if the curvature of the nanotube changes, the atomic orbitals overlapping also varies and the exchange parameter needs to be recalculated, according to the expression (2)

$$J_t = \frac{c}{a} J_s \tag{2}$$

In the nanotube longitudinal section, periodical boundary conditions were assigned for considering the fact that in real nanotubes, the diameter is smaller than the length. Moreover, in the nanotube cross section free boundary conditions were established. Finally statistical averages were performed employing 2×10^4 Monte Carlo steps.

The magnetic susceptibility χ by using the Monte Carlo results was obtained, according to the (Eq. 3)

$$\chi = N^{-1} \frac{1}{k_b T} (\langle m_i^2 \rangle - \langle m_i \rangle^2) \tag{3}$$

where N is the number of magnetic ions in the system and $\langle m_i \rangle$ is the mean magnetization at the longitudinal-direction per spin. The specific heat C is obtained from the energy fluctuation (Eq. 4).

$$C = N^{-1} \frac{1}{k_b T} (\langle E^2 \rangle - \langle E \rangle^2) \tag{4}$$

where $\langle E \rangle$ is the mean energy per spin.

3. Results and discussion

Figure 2 shows the magnetization per magnetic site and the magnetic susceptibility for a nanotube with diameter $m=20$. Typical ferromagnetic behavior is observed; at low temperatures, magnetization is high due to the spins ordering is not affected by the low entropy. Furthermore, the magneto-crystalline anisotropy along the longitudinal direction of the nanotube plays a very important role. As the temperature is

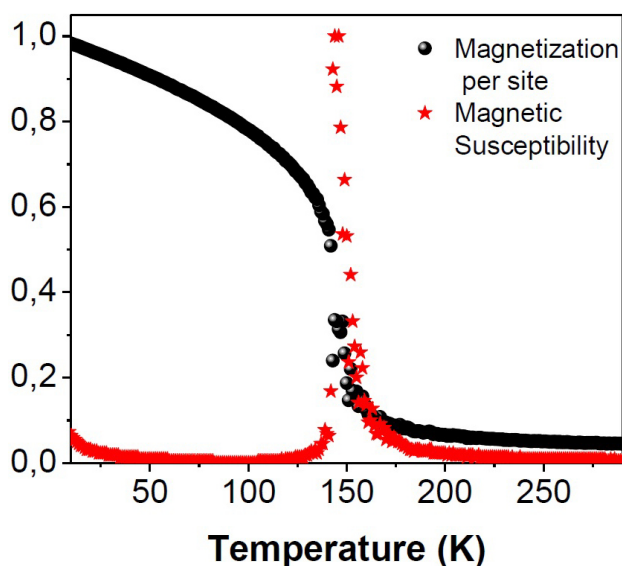


FIGURE 2. Magnetization per magnetic site and magnetic susceptibility in normalized unites as a function of temperature for a nanotube with $m=20$.

increased, the magnetization decreases presenting an inflexion point. It means that nanotubes undergo a magnetic phase transition from ferromagnetic to paramagnetic state. After the transition point, the temperature plays the most important role in the magnetic properties, as a result of the increment in the entropy [19]. Magnetic susceptibility measured from the fluctuations in the magnetization shows a maximum at the critical point, where the magnetic system changes its magnetic behavior from ferromagnetic to paramagnetic.

Ferromagnetic energy as a function of temperature is presented in Fig. 3. As is expected, it increases, tending to the saturation [20]. The specific heat curve has a well defined lambda shape which is a characteristic of this kind of magnetic transitions [21].

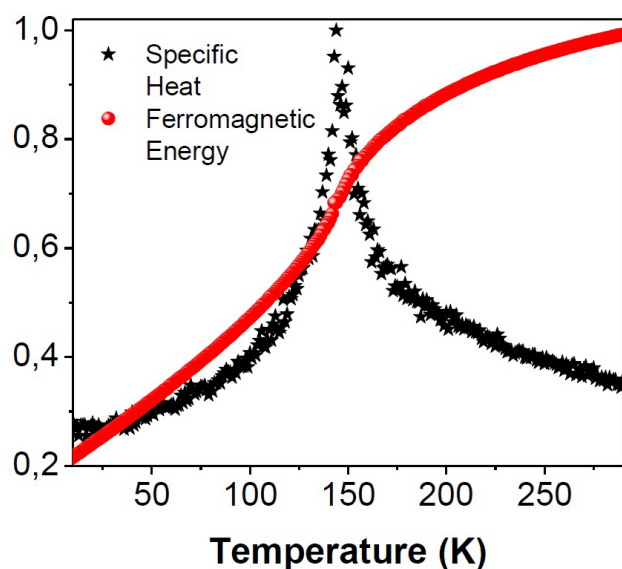


FIGURE 3. Ferromagnetic energy and specific heat in normalized units as a function of temperature for a nanotube with $m=20$.

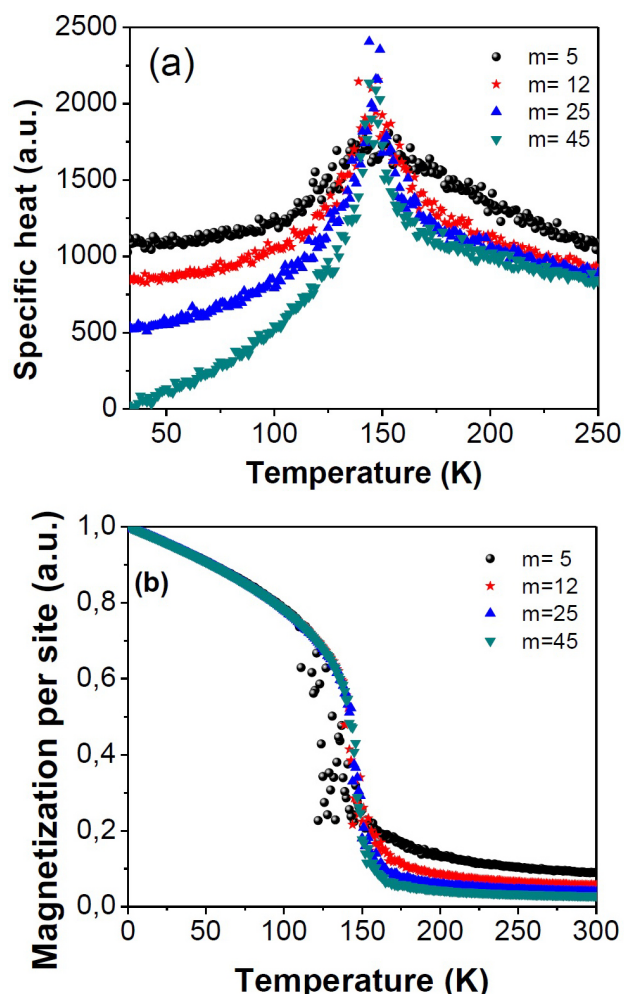


FIGURE 4. a) Specific heat curves as a function of temperature for nanotubes of different diameter b) magnetization curves as a function of temperature for nanotubes of different diameter.

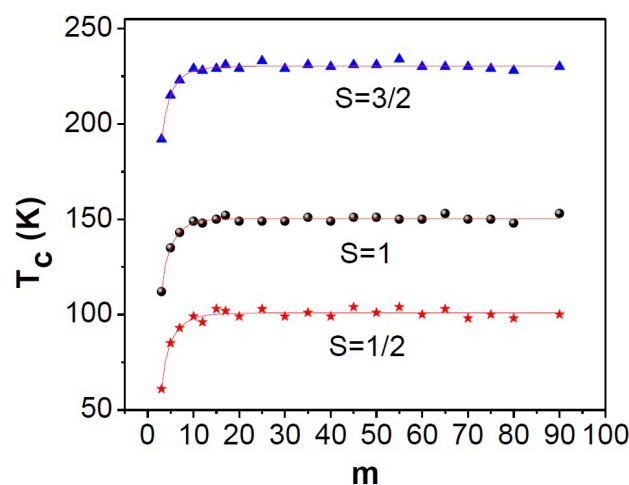


FIGURE 5. Critical temperature as a function of the number m .

Specific heat curves for nanotubes of different diameters were plotted in Fig. 4 a). A visible characteristic observed in this figure due to the finite size effect is the tendency of

peaks to be sharper as the diameter increases. It produces a more abrupt ferromagnetic to paramagnetic phase transition. Figure 4 b) shows magnetizations curves for some nanotube diameters (m). For the smallest diameter the magnetization curve presents more data dispersion in the zone of the transition temperature due the effects of a low quantity of magnetic ions.

Figure 5 illustrates the Curie temperature versus the diameter of the nanotube for three different quantum spins values. When the diameter rises, the critical temperature increases, reflecting that the collective effect of adjacent ions is increased and the fluctuation effect is neglected as the number of spins in the cross section (m) rises. This figure also shows that the slop of each curve decreases with m , and the critical temperature value finally approaches to a 2D monolayer as m tends to infinity. In addition, from Fig. 5, under fixed diameter, the Curie temperature increases as the quantum spin number is higher [18].

4. Conclusions

Magnetization per magnetic site, magnetic susceptibility, ferromagnetic energy and specific heat curves were obtained for a system of atoms ordered as a nanotube by means of

a computational model based in the Monte Carlo method and a classical Heisenberg Hamiltonian. These curves describe the transition from ferromagnetic to paramagnetic phase as a function of temperature for nanotubes of different diameters. Results show the evolution of the Curie temperature with the diameter until reaching a saturation temperature which is in agreement with the transition temperature of a 2D monolayer. Similar behavior was observed in works reported by Konstantinova and B.-Z. Mi *et al* in magnetic properties of nanotubes, when the system presents values of anisotropy and exchange parameters in the same order of magnitude. The computational model reveals an appreciable change in the magnetic properties as the diameter of the tube tends to be smaller; according to the finite size scaling theory.

Acknowledgements

This work was supported by La Dirección de Investigaciones de la Universidad Nacional de Colombia Sede Manizales – DIMA, under the Project 11714 approved in La convocatoria para el apoyo a tesis de posgrado and the project number 10719. This work was also partially supported by Research Project SIP-20060859.

-
1. S. Iijima, *Nature* **354** (1991) 56.
 2. S. Sun, C.B. Murray, D. Weller, L. Folks, and A. Moser, *Science* **287** (2000) 1989.
 3. R. Skomski, *J.Phys. Condens. Matter* **15** (2003) R841.
 4. S. Khizroev, M. H. Kryder, D. Litvinov, and D.A. Thompson, *Appl. Phys. Lett.* **81** (2002) 2256.
 5. Y. Xu, D.S. Xue, J.L. Fu, D.Q. Gao, and B. Gao, *J. Phys. D: Appl. Phys.* **41** (2008) 215010.
 6. Dong Zhou, Li-heng Cai, Fu-shen Wen, and Fa-shen Li, *Chin. J. Chem. Phys.* **20** (2007) 821.
 7. F.S.Li, D. Zhou, T. Wang, Y. Wang, L.J. Song, C.T. Xu, *J. Appl. Phys.* **101** (2007) 014309.
 8. W.A. Alves, R.H.A. Santos, A. Paduan-Filho, C.C. Becerra, A.C. Borin, and A.M.D.C. Ferreira, *Inorg. Chem.* **357** (2004) 2269.
 9. M.A. Bizeto, W.A. Alves, C.A.S. Barbosa, A.M.D.C. Ferreira, and V.R.L. Constantino, *Inorg. Chem.* **45** (2006) 6214.
 10. E. Konstantinova, *J. Mag. Mag. Mat.* **320** (2008) 2721–2729.
 11. Z.K. Wang *et al.*, *Phys. Rev. Lett.* **94** (2005) 137208.
 12. A.P. Chen, N.A. Usov, J.M. Blanco, and J. Gonzales, *J. Magn. Magn. Mater.* **316** (2007) e317.
 13. Jehyun Lee, Dieter Suess, Thomas Schrefl, Kyu Hwan Oha, and Josef Fidler, *J. Magn. Magn. Mater.* **310** (2007) 2445.
 14. P.Landeros, S. Allende, J. Escrig, E. Salcedo, D.Altbir, *Appl. Phys. Lett.* **90** (2007) 102501.
 15. P. Landeros, O.J. Suarez, A. Cuchillo, and P. Vargas, *Phys. Rev. B* **79** (2009) 024404.
 16. T.K. Das, and M.G. Cottam, *J. Appl. Phys.* **103** (2008) 07B104.
 17. S. Allende, J. Escrig, D. Altbir, E. Salcedo, and M. Bahiana, *Eur. Phys. J.B.* **66** (2008) 37.
 18. Bin-Zhou Mi, Huai-Yu Wang, Yun-Song Zhou, *J. Mag. Mag. Mat* **322** (2010) 952-958.
 19. Charles Kittel, *Introduction to Solid State Physics*, (Wiley, New York 1996).
 20. P. Papon, J. Leblond, and P.h. Meijer, *The Physics of Phase Transitions*, second edition, (Springer, Berlin, 2006).
 21. J. Mazo-Zuluaga, and J. Restrepo, *Physica B* **384** (2006) 224-226.