Magnetic phase diagram of a nanocone

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Abstract. In this work we analyze the magnetic properties of truncated conical nanoparticles. Based on the continuous magnetic model we find expressions for the total energy in three different magnetic configurations. Finally, we calculate the magnetic phase diagram as function of the geometrical parameters.

1. Introduction
The magnetic nano-objects have been deeply investigated during the last decades. Besides, the basic scientific interest in the magnetic properties of these systems, there is evidence that they might be used in the production of new technological applications. One of the main points in the study of such systems concerns the internal magnetic structure of the nanoparticles as a function of their shape and size. For example, in the case of cylindrically shaped particles produced by electrodeposition, the internal arrangements of the magnetic moments have been identified as being close to one of the following three idealized characteristic configurations: ferromagnetic with the magnetization parallel to the basis of the cylinder ($F_1$), ferromagnetic with the magnetization parallel to the cylinder axis ($F_2$), and a vortex state, in which most of the magnetic moments lie parallel to the basis of the cylinder $V$ [1, 2].

On the other hand, theoretical determination of the configuration of lowest energy of particles in the size range of those currently produced, based on a microscopic approach and using present standard computational facilities, is out of reach. The reason is the exceedingly large number of magnetic moments within such particles, which may exceed $10^9$. Recently, d’Albuquerque e Castro et al.[3] have proposed a scaling technique for determining the phase diagram giving the configuration of lowest energy among the three abovementioned characteristic magnetic configurations. This scaling technique has been applied to the determination of the phase diagram of cylindrically shaped [3] and truncated conical [4] particles.

Recently, was proposed a computational scheme to determine the complete demagnetization tensor field and the volumetric demagnetization factors for arbitrary shapes [5]. Once these quantities are available, it is often straightforward to determine the dependence of the energetics of the magnetic system on the shape parameters, and with this method was calculated the...
phase diagram for a magnetic nanoring [6]. Alternatively, using the continuous approach was calculated the stability of magnetic configurations and phase diagrams of cylindrically shaped and ring shaped [7, 8].

The goal of this article is presented the theoretical calculation of truncated conical particles using the continuous approach. In particular, we calculate the magnetic phase diagram. The paper is organized as follows: In Sec. II, the theoretical model is presented and the results are discussed. Finally, conclusions are presented in Sec. III.

2. Theoretical model and Results

Geometrically, nanocones are characterized by their radius, $R_1$ and $R_2$ and length, $H$ as shown in Fig.(1). In order to describe this problem we use a continuous approach and adopt a simplified description in which the discrete distribution of magnetic moments in each cone is replaced with a continuous one, defined by a function $M(r)$ such that $M(r)\delta v$ gives the total magnetic moment within the element of volume $\delta v$ centered at $r$. We recall that is generally given by the sum of three terms corresponding to the magnetostatic, the exchange and the anisotropy contributions. Here we are interested in soft or polycrystalline magnetic materials, in which case the anisotropy is usually disregarded [9].

![Figure 1. Schematic shape of nanocone](image)

Therefore, the total energy can be cast:

\[
E_T = \frac{\mu_0}{2\nu} \int \mathbf{M}(r) \cdot \nabla U(r) dv + \frac{A}{\nu} \int (\nabla m_x)^2 + (\nabla m_y)^2 + (\nabla m_z)^2) dv
\]

where $A$ is the exchange stiffness constant, $\nu$ the volume given by $\nu = \frac{\pi}{3}[H^2 + (R_1 - R_2)^2]^{1/2}(R_1^2 + R_1 R_2 + R_2^2)$ and the scalar magnetic potential $U(r)$ is can be expresses as

\[
U(r) = -\frac{1}{4\pi} \int \frac{\nabla \cdot \mathbf{M}(r')}{|r - r'|} dv' + \frac{1}{4\pi} \int \frac{\mathbf{n}' \cdot \mathbf{M}(r')}{|r - r'|} ds'.
\]

where $ds$ is the element of surface. In our case the three magnetic configuration are: ferromagnetic with the magnetization parallel to the basis of the cylinder ($F1$), ferromagnetic
with the magnetization parallel to the cylinder axis (F2), and a vortex state, in which most of the magnetic moments lie parallel to the basis of the cylinder (V); so the mathematical structure of magnetization field are: \( M_0 \hat{x}, M_0 \hat{y} \) and \( M_0 \hat{z} \), respectively, being \( M_0 \) a constant.

We note that, for the considered magnetic configurations in the scalar magnetic potential the volumetric contributions are zero; hence we must only calculate the surface terms, and it can be expresses as the contribution of three element terms: the top \( ds_1 = \rho d\rho d\varphi \), the shell \( ds_L = (R_2 - z\tan(\alpha))d\rho dz(\rho - \tan(\alpha)) \), and the bottom \( ds_2 = -\rho d\rho d\varphi \); in addition, the constrain on the surface is given by \( \rho = (R_2 - z\tan(\alpha)) \), being \( \tan(\alpha) = \frac{R_2 - R_b}{R_2 - R_1} \).

Let us start our analysis calculating the total energy for the vortex configuration (V). In such case, the only contribution correspond to the exchange energy; we assume a cut-off which represent the lattice parameter, \( r \). Consequently:

\[
E_T^{(V)} = 2\pi AH[\ln \frac{R_1}{r} + \frac{R_2}{R_2 - R_1} \ln \frac{R_2}{R_1} - \frac{1}{2}]
\]

(3)

Now, let us calculate the ferromagnetic configurations, in these cases the exchange contribution is zero. Therefore, the total energy for the in-plane configuration (F1) can be cast

\[
E_{d_x} = \mu_0 M_0^2 \sum_{n=0}^{\infty} D[R_2, R_1, H, n] I_n
\]

(4)

where

\[
D[R_2, R_1, H, n] = \frac{H^2\pi}{(R_2 - R_1)^2 2^{n/2} n!} \left( \frac{5/4}{2} \right)^n (3/4)^n (2)_n
\]

(5)

\[
I_n = \int_{R_1}^{R_2} \rho' d\rho' \int_{R_1}^{R_2} \rho d\rho \times 1 \left( \rho' \rho \right)^{1/2} \left[ 1 + \frac{(\rho' - \rho)^2}{2\rho\rho'} \right] \left[ 1 + \frac{H}{R_2 - R_1} \right]^{2n + 3/2}
\]

(6)

with \( (x)_n = \frac{\Gamma(x+n)}{\Gamma(x)} \) and \( \Gamma(x) \) the Gamma function. In addition, in the case of out-of plane (F2) configuration we obtain: **Magnetización en Z:**

\[
E_{d_z} = \frac{\mu_0 M_0^2}{8\pi} [\frac{16\pi}{3} (R_3^2 - R_1^2) + 2 \sum_{n=0}^{\infty} X[n] (I_{2n} - \frac{P[R_1, R_2, H, n]}{X[n]} - I_{4n} + \frac{I_{5n}}{2})]
\]

(7)

where

\[
X[n] = \frac{4\pi \Gamma[1/2]^2 (3/4)_n (1/4)_n}{2^{1/2}(1)_n}
\]

(8)

\[
P[R_1, R_2, H, n] = \frac{\pi^2 R_2^2 R_1^4 \Gamma[1 + 2n]}{Hn! \Gamma[2 + n]} \times F_{21}[n - (1 + n); 2; \frac{R_1^2}{R_2^2}(-\frac{R_2^2}{4H^2})^n]
\]

(9)

\[
I_{2n} = \int_{R_1}^{R_2} \rho d\rho \int_{R_1}^{R_2} \rho' d\rho' \times 1 \left( \rho' \rho \right)^{1/2} \left( \frac{2\rho\rho'}{R_2 - R_1} \right)^2 + \rho^2 + \rho'^2 \right]^{2n + 1/2}
\]

(10)

\[
I_{4n} = \int_{R_1}^{R_2} \rho d\rho \int_{0}^{R_1} \rho' d\rho' \times 1 \left( \rho' \rho \right)^{1/2} \left( \frac{2\rho\rho'}{R_2 - R_1} \right)^2 + \rho^2 + \rho'^2 \right]^{2n + 1/2}
\]

(11)
\[ I_{5n} = \int_{R_1}^{R_2} \rho d\rho \int_{R_1}^{R_2} \rho' d\rho' \frac{1}{(\rho' / \rho)^{1/2}} \times \frac{1}{[1 + \frac{(\rho' - \rho)^2}{2 \rho \rho'} (1 + \frac{H}{R_2 - R_1})^2]^{2n+1/2}} \]  

(12)

\( F_{21}(a, b; c; d) \) being the usual Hypergeometric function.

**Figure 2.** Phase diagram for magnetic nanocone.

The integrals \( I_n \), \( I_{2n} \), \( I_{4n} \) and \( I_{5n} \) must be solve numerically and in order to find numerical precision we use the Monte-Carlo integration method with 35 points for maximum recursion.

Obviously, once the numerical calculations for all total energies have been obtained, is possible to make the phase diagram; and it indicates regions where configurations are relatively more stable. The main result is displayed in Fig.(2), where we plot the diagram of the length, \( H \), as a function of bigger radius \( R_2 \) at \( R_1 = 10[\text{nm}] \). We find that, for a short radius and length the system prefer the \( F1 \) configuration, for a short radius and high length the system prefer \( F2 \) configuration and in other case the system prefer the \( V \) configuration. We remark that, our calculations are in good agrement with the experimental data [2] and Monte-Carlo simulations [4].

3. Conclusions

In the present work, the magnetic properties of of truncated conical nanoparticles is studied. We determine the stability thresholds of vortex, in-plane and out-of-plane configurations. Beside, our results are in good agrement with the experimental data.

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