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ACCEPTED MANUSCRIPT

Magnetic properties of crystalline nanoparticles with different sizes and shapes.

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The effects of shape and finite size on the physical behavior of nanostructured antiferromagnetic particles are investigated. They were modeled as ellipsoidal systems which preserve the crystalline structure of the correspondent bulk material. In our analysis we consider nanoparticles composed by magnetic ions which are themselves insensitive to the presence of surfaces and/or interfaces. Results are shown for structures similar to MnF_2 and NiO crystals. Special attention is given to these last once their singular magnetic arrangement, as well as, their use at different technological and/or biomedical applications, has motivated intense experimental studies at different laboratories. We use the parameters that describe the correspondent bulk material to discuss the magnetic behavior of these particles for different volumes and shapes.

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Keywords: magnetic particles; nanostructured magnetic particles; hysteresis loops; dynamical behavior

I. INTRODUCTION

The use of particles with size in the nanometric scale in the everyday life has increased continuously and, in particular, magnetic nanoparticles have been used for applications that go from the use in the development of reliable large data storage devices^{1,2} to the use in medical procedures that require non-invasive techniques for imaging and/or localized therapy of serious diseases³⁻⁵. Despite the motivation and the large number of papers dealing with these systems, there are several properties that are not fully understood (as the exchange bias effect $^{6-9}$) and are still challenges for those working in this field. The demand for a better understanding of these systems comes from the fact that in recent years the development of growth techniques has allowed the preparation of this kind of particle with well controlled geometric and structural characteristics. It is well known that physical properties of small systems are modified by the breaking of the lattice symmetry, as well as, broken bonds due to the presence of surface. This requires a major effort in the search for better comprehension of the consequences of the presence of surfaces in systems with size in this domain. Moreover, since several properties depend on these geometric characteristics, the rapid development of well controlled growth techniques also allows one to prescribes that very soon will be possible the obtaining of particles to fit a large range of needs.

Most of low dimension magnetic systems studied in the last decades were very thin films. To them, the border effects were not relevant and the main modifications of the physical properties came from the break of symmetry in one direction. In some sense, magnetic nanoparticles might be seen as a thin magnetic film with relevant border effects. This fact gives to these systems a much richer variety of externally controlled properties that can be used to adapt them to different applications. Useful approaches to study these nanoparticles are reported by several authors (see e.g., Zysleka et al. 10 and Liu Zhao-Sen et al. 11). A good review on the procedures and approaches used to study small magnetic particles can be found in the papers of R.H. Kodama and co-authors 12-14.

The main goal of this work is to discuss the changes imposed by surfaces on the magnetic properties of small nanostructured antiferromagnetic particles. We start modeling the particles as a collection of ions with well localized positions in the crystalline structure. Moreover, we assume that the ions have well defined magnetic moments, which are not sensitive to their location. However, it is assumed that their orientation is the result of the competition of all magnetic interactions present in the system. We start Section II calculating the magnetization of nanoparticles resulting from nano portions of MnF_2 crystals. This material was chosen not only for being one of the most studied, but also because it can be seen as a prototype of the antiferromagnetic materials. The results pave the way for the understanding of more complex systems. This calculation is followed by a more thorough study of NiO nanoparticles. In NiO crystals, each magnetic moment of its fcc type II crystalline structure has twelve nearest neighbors and six next nearest neighbors and, in the bulk configuration can be seen as a collection of ferromagnetic planes coupled antiferromagnetically. We investigate the influence of the break of symmetry introduced by the surface of the particle on the hysteresis loop. The magnetic resonances are also in-

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