

## MICROSCOPIC ORIGIN OF EXCHANGE BIAS IN INVERTED CORE/SHELL MAGNETIC NANOPARTICLES

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The exchange bias (EB) phenomenon has been reported in a variety of nanoparticle systems with core/shell structure until its first report in the 50's. In most of the cases, this phenomenology has been observed in the paradigmatic case of a nanoparticle consisting of a ferromagnetic (FM) core surrounded by an antiferromagnet (AFM) with Néel temperature ( $T_N$ ) lower than the Curie temperature ( $T_C$ ) of the FM. However, there have been recent studies [1] reporting the observation of EB in nanoparticles with doubly inverted composition: an AFM core (MnO) surrounded by a ferrimagnetic shell ( $Mn_3O_4$ ) and with a  $T_C$  much lower than the  $T_N$  of the core. These unusual observations, together with the peculiar magnetic properties of these systems [1], remain a challenge for the current proposed models of EB in nanoparticles.

We present results of Monte Carlo (MC) simulations based on a classical Heisenberg model of lattice spins for a core (AFM)/shell (FM) nanoparticle in which the values of microscopic parameters such as anisotropy  $K$  and exchange constants  $J$  can be tuned in the core, shell and at the interfacial regions, offering new insight on the microscopic origin of the experimental phenomenology [2]. To this end, we have computed low temperature equilibrium magnetic configurations (see Fig. 1) in the presence of a magnetic field and at zero field for different values of the  $K$ 's and  $J$ 's in order to study the magnetic order established at the core/shell interface, which is essential to understand EB. We have also simulated hysteresis loops after field cooling as a function of the exchange coupling at the interface (see Fig. 2) and  $K$  for a range of particle diameters similar to the experimental systems. The simulated loops display shifts along the field axis with a nonmonotonous dependence on the core diameter in qualitative agreement with the experimental observation. A detailed analysis of the interfacial spin configurations along the loops have allowed us to quantify the magnitude of the loop shifts with striking agreement with the macroscopic observed values and to give compelling evidence of the relevant role of the uncompensated net magnetization at the interface to explain the observed phenomenology.

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### References:

- [1] G. Salazar-Alvarez *et al.*, J. Am. Chem. Soc. 129 (2007) 9102; A. E. Berkowitz *et al.*, Phys. Rev. B 77 (2008) 024403.
- [2] O. Iglesias, X. Batlle and A. Labarta, Phys. Rev. B 72 212401 (2005), J. Nanosci. Nanotechnol. 8 (2008) 2761.

Figures:

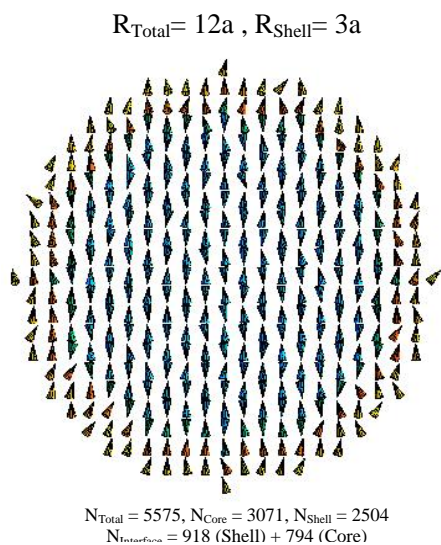


FIGURE 1: Magnetic configuration of a nanoparticle with AFM core/FM shell structure after a field cooling process.

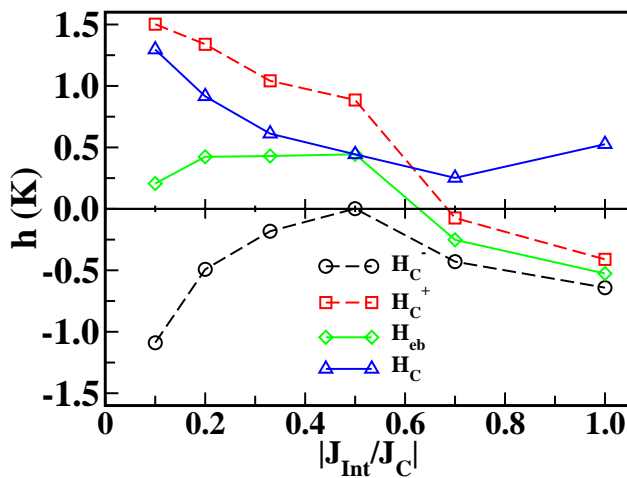


FIGURE 2: Dependence of the coercive field and exchange bias fields on the exchange coupling constant at the interface for antiferromagnetic interfacial coupling.