Magnetism at nanoscopic scale : numerical simulation and applications

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Introduction Magnetisation reversal in thin layers plays a key role in magnetic recording and has recently attracted much attention, particularly for materials exhibiting high magnetocrystalline anisotropy.

Among these materials, FePt in its $L1_0$ phase is a promising candidate for high density magnetic recording systems with giant anisotropy of about 5.10^6 J.m⁻³.

Magnetisation reversal is often linked to domain wall displacement in the layer. This motion can be influenced by the interaction with structural defects such as antiphase boundaries or extended defects called micro-twins, which appear preferentially in ordered FePt[1].

Modelling In order to correctly simulate domain wall pinning, the atomic structure has to be taken into account. We have developed an algorithm that minimizes magnetic energy using the Heisenberg model. Energy terms taken into account are exchange energy, anisotropy, dipolar energy and energy due to an applied field.

The correct handling of the anisotropy in structural defects was carried out by using Néel's model, which considers the anisotropy of an atomic site as the result of its close environment.

The computation of the dipolar term is the real bottleneck in atomistic simulations given that it is a long range interaction. Therefore, without any approximation, computing this term requires a time proportional to $O(n^2)$ where n is the total number of spins.

In order to speed up the calculation of this term, we adapted a Fast Multipole Method (FMM) [2] to atomic magnetism. This kind of method is based on the multipolar expansion of the potential (coulombic, gravitational, etc.) to gather particles. It can achieve the computation in a time proportional to the number of atoms with a precise control on the error made by truncating the expansion.

Results This algorithm was used to study the pinning of a domain wall by a micro-twin (figure 1). Computations have shown a strong pinning by this type of defect : for a micro-twin constituted of 6 atomic layers, the depinning field is about 2.5 T.

In fact, once the domain wall is pinned into the micro-twin, the application of a field to move the wall on the left or on the right shows that depinning is easier in the opposite direction of the propagation (B = 1.9 T, whereas a field of 2.8 T is necessary in the other direction). Therefore the configuration is asymmetric and the depinning field of a domain wall in a given direction gives us information on the direction of propagation before the wall reaches the defect.

References

- [1] J. P. Attané et al., *Magnetic Domain Wall Propagation unto the Percolation Threshold* across a Pseudorectangular Disordered Lattice, Phys. Rev. Lett., **93**, 2004
- [2] H. Cheng, L. Greengard and V. Rokhlin, *A Fast Adaptative Multipole Algorithm in Three Dimensions*, J. Comp. Phys., **155**, 1999

Figures :

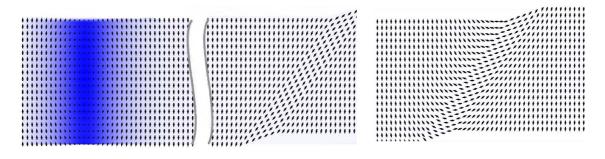


Figure 1: Domain wall far from the micro-twin (left) and pinned into this defect (right); the system is invariant along the normal of the figure's plane.