Numerical investigations of micromagnetic structures

Summary of the Ph.D. Thesis

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1. Introduction

In the 1960's, the micromagnetics became a substitute for the domain theory, where the domains and the domain walls are treated together. The first complete formulation of the micromagnetic method was due to Brown [1963], with an a priori conclusion: "clearly micromagnetics is not yet ready to eject domain theory from the position that it now holds by default. But micromagnetics can at least formulate explicitly and attack honestly problems that domain theory evades". The effectiveness of micromagnetics started ten years after Brown's micromagnetic formulation with the advent of relatively high-speed computers.

The aim of micromagnetics is to get information on the magnetic moment orientation distribution in micron-sized or submicron-sized objects, i.e. on magnetic domains and domain wall structures. Whereas experimental techniques of magnetic domain observations (Bitter patterns, Kerr Microscopy and Magnetic Force Microscopy) provide information on the surface magnetic orientation only, the micromagnetic simulations are capable of describing the internal magnetic moment configurations as well. In addition, micromagnetic calculations enable us to compare the energy of various magnetic configurations which cannot be detemined experimentally.

Mostly, the micromagnetic community focuses on understanding the magnetization processes of materials and devices used in magnetic information storage, especially in the latest development of patterned storage media at the edge of the superparamagnetic limit. Micromagnetics allowed to design the $1GByte/inch^2$ hard disks, which are under laboratory test (Seegate Company, Pittsburg) and the first magnetic random access memory (MRAM, Anthony S. Arrott), which is already in the productional phase. Another interesting problem is the optimization of the $(BH)_{max}$ energy in hard-soft nanocomposite materials.

But micromagnetics can also be used to understand and design new types of soft magnetic nanocrystalline alloys or to calculate the magnetization structure of fine particles in the nanosized regime, having actuality because of their importance in biomedical appications.

It is worth mentioning that whereas over the last hundred years (dated arbitrarily from Ewing) the physical properties of magnetic materials (Curie temperature and saturation magnetization) could hardly be improved, the technical magnetization parameters (coercive field, permeability, power loss) could be improved radically, by several orders of magnitude.

2. Objectives

The micromagnetic calculations became more and more important both for basic science and industrial applications. It helps us understand the magnetization processes and design new materials for a given application.

My first objective was to study the domain wall structures in Permalloy films, used in magnetic read-write heads. The requirements of nowadays are to have a large bit density and a fast reading or writing process. These are contradictions because the large bit density requires small magnetic head, but the small head means that the magnetization process is driven by Néel walls. The mobility of a Néel wall is smaller than that of a Bloch wall. Due to the interaction of Bloch and Néel walls three-dimensional, so-called cross-tie walls appear in the nanometer range, with a Vertical Bloch Line (VBL) in the middle. The interaction of VBLs is slowing down the read-write process. Two questions had to be answered:

- what is the film thickness at which the Bloch to Néel wall transition occurs?
- what is the energy of the experimentally observed cross-tie walls as compared to the simple walls at the Bloch to Néel wall transition thickness?

My second objective was to study the nanocrystalline (nc) soft magnetic materials. The exchange-averaging model of Herzer[1990] based on the random walk considerations to derive the effective anisotropy of a nanocrystalline material is a phenomenological model. The aim of the work was to validate this model by micromagnetic calculations. The micromagnetic calculations however can be done on small-sized samples only, where the strong demagnetizing effects are unavoidable. The Herzer model is implicitly assuming an infinite-sized sample where the balance of exchange and anisotropy is taken into account only. For a small-sized sample, the object of micromagnetic calculations, beside these two energies the magnetostatic stray field energy can't be neglected. The latter is equivalent with a strong, uniaxial shape anisotropy. In addition, we would like to follow the averaging out of the fluctuations of local magnetocrystalline anisotropies.

The third objective was to study the magnetic structure (monodomain-vortex transition) of fine particles and to develop a method for the determination of their size distribution. The magnetization of non-interacting nanoparticles (well above the superparamagnetic transition temperature) follow a Langevin curve of magnetization, more precisely a superposition of Langevin functions. The shape of this curve depends only on the distribution of particle sizes and, hence, it can be used in magnetic or "Langevin granulometry" to determine this distribution. These magnetic nanoparticles have actuality because of their importance in biomedical applications.

3. Computational methodology

3.1. Micromagnetics

In micromagnetics, domain walls and domain wall structures are represented by a continuous function of the magnetization, constant in magnitude but changing in direction from position to position. The dynamics of each elementary cell (volume) of magnetization, also called dipole moment or magnetic spin, is described by the non–linear Landau-Lifshitz-Gilbert equation

$$\frac{d\vec{M}}{dt} = -\frac{\gamma}{1+\alpha^2}\left[\vec{M} \times \vec{H_{eff}} + \frac{\alpha}{M_s}\vec{M} \times \left(\vec{M} \times \vec{H_{eff}}\right)\right], \qquad (1)$$

where the H_{eff} is the effective field comprising the anisotropy, exchange, demagnetization and external fields, γ is the gyromagnetic ratio and α is the Gilbert damping parameter. In order to capture the continuous character of the magnetization distribution, the simulation of walls and wall structures requires that the magnetic sample be configured in a finely discretized lattice such that each node in the lattice has uniform magnetization. The magnetization dynamics of walls and domain wall structures are then investigated by solving numerically the LLG equation at each point in the lattice. Several hundred thousand grid points are necessary to configure magnetic structures in this discrete lattice. The numerical resolution of the LLG at each grid-point becomes time consuming on conventional computers.

Each elementary cell is represented by a unit magnetization vector $\vec{m}(m_x, m_y, m_z)$ and corresponds to a uniform magnetic volume defined by the exchange parameter A, anisotropy constant K, saturation magnetization M_s, gyromagnetic ration γ and the damping parameter α. These are the input parameters for the calculation process. The elementary cell size depends on the material parameters.

The initial state for the simulation is usually different for each considered problem. In some cases, analytical solutions are taken for initial state or just a random configuration for the unit magnetization vector.

3.2. Langevin granulometry

In the case of non–interacting superparamagnetic particles having a size (i.e. magnetic moment) distribution, the magnetization curves taken at different temperatures collapse to a single curve in a $M(H,T)/M_s(T)$ vs. $M_s(T)H/T$ plot, which is normally a superposition of Langevin functions. The shape of this curve depends only on the distribution of particle sizes and hence it can be used as a magnetic or "Langevin granulometer" to determine this distribution. Although several other techniques are available for the determination of particle size distributions, such as transmission electron microscopy, small angle neutron scattering, etc., the magnetic method is easier to perform experimentally. Of course, this technique presents the same difficulty as many other problems in data evaluation, namely the physical system uniquely determine the measured data but the inverse problem of deriving the parameters of the physical system from the data is ambiguous.

The magnetization of a sample that contains a distribution of particle types is given by

$$M(H,T) = \sum_{i=1}^{N} w_i \mu_i \mathrm{Lang}\left(\frac{\mu_0 \mu_i H}{k_B T}\right) \tag{2}$$

where $w_i = w_i(\mu_i)$ is the number of particles of type i, per unit volume, each carrying the magnetic moment equal to μ_i.

The task is to determine the distribution of the magnetic moment, $w_i(\mu_i)$ – directly related to the particle size – from the experimental magnetization curve, $M(H,T)$.

4. New scientific results

1. A more accurate thickness value for the Bloch–to–Néel wall transition was established for Permalloy film. Instead of the previously determined value of 80–90 nm ([Labonte, 1969][Hubert, 1998]), we obtained 30–35 nm [1]. In addition, we have shown that symmetric Bloch walls exist down to 35 nm [1] instead of the previously reported limit of 100 nm [Labonte, 1969]. These findings have relevance in designing read–write heads of hard disks based on Permalloy thin films.

2. By studying a multitude of coexistent Bloch and Néel walls in Permalloy thin films in the transition thickness range (10-70 nm), cross-tie walls have been found [2] in agreement with earlier experimental results [Hubert, 1998][Huber, 1958]. The occurrence of a cross-tie wall structure reflects a change in the nature of the walls visible at the surface: the Néel wall rotation at the surface is stopped after 90° and a vertical Bloch line appears where two C-shaped domain walls of opposite chirality meet [Redjdal, 1998] and the magnetic transition continues with a Néel wall rotation in the same sense. The simulation of the cross-tie wall structure at the Néel–to–Bloch transition thickness provides a detailed visualization and quantitative data on transition widths and wall energy[2]. Such calculations are the only source of information about the internal domain wall structures because the experimental observations are restricted to the surface of the sample. These calculations are necessary to design the magnetic storage devices, i.e. the shpae and the size of the read–write heads.

3. We have found by micromagnetic calculations that the domain wall thickness changes as the inverse third power of the grain size [3], in agreement with the Herzer formula describing the exchange softening in nanosized region. These

calculations provide a proof for the scaling considerations used in deriving the random anisotropy model.

4. We have calculated, for the first time, by micromagnetics the critical diameters for monodomain–to–vortex transition in sphere-like soft magnetic fine particles [4]. In agreement with the earlier analytical calculations of Brown [1968], we have found two critical diameters D_{mono} and D_{vortex} which refer to the pure monodomain (the [0,D_{mono}] interval) and pure vortex structure (above D_{vortex}). Moreover, the structure between D_{mono} and D_{vortex} could be cleared up, which was missing from the literature: in this region, a hard–axis–oriented [4] vortex state was found instead of the "normal" easy–axis–oriented vortex. These calculations are informative for those working in biomedical applications, i.e. biological markers, hypethermal treatments.

5. A software was developed based on genetic algorithm for extracting the magnetic moment distribution from superparamagnetic magnetization curves [5]. Though many other methods have been used so far, this software available now on the author's website [http://www.szfki.hu/˜attilak/software.html] is the only reliable method of processing superparamagnetic curves, making possible for the first time real Langevin granulometry through magnetization measurements, either for a single lognormal or multi-modal distributions.

5. References

[Brown, 1963]: W.F. Brown, Jr., 1963 *Micromagnetics* John Wiley & Sons, New York.

[Ewing, 1885]: J.R. Ewing, 1885 *Philosophical Transactions of the Royal Society – Part II.* pp. 523-640, plus plates 57-68.

[Herzer, 1990]: G. Herzer, 1990 *IEEE Trans. Magn.* **26** 1397.

[Labonte, 1969]: A.E. Labonte, 1969 *J. Appl. Phys.* **40** 2450-2458.

[Hubert, 1998]: A. Hubert, R. Schäfer *Magnetic Domains* ISBN 3-540-64108-4 Springer p. 110.

[Huber, 1958]: E.E. Huber, JR., D. O. Smith, and J. B. Goodenough, 1958 *J. Appl. Phys.* **29(3)** 294-295.

[Redjdal, 1998]: M. Redjdal, Ph.D. thesis (Boston University)

6. Publications related to the Ph.D. work

[1] T. Trunk, M. Redjdal, **A. Kákay**, M.F. Raune and F.B. Humphrey, *Domain wall structure in Permalloy films with decreasing thickness at the Bloch to Néel transition*, 2001 *J. Appl. Phys.* **89(11)** 7606-7608.

[2] M. Redjdal, **A. Kákay**, M.F. Raune and F.B. Humphrey, *Cross-tie walls in thin Permalloy films*, 2002 *IEEE Trans. Magn.* **38(5)** 2471-2473.

[3] **A. Kákay** and L.K. Varga, *Micromagnetic simulation of random anisotropy model*, 2004 *J. Magn. Magn. Mat.* **272-276** 741-742

[4] **A. Kákay** and L.K. Varga, *Monodomain critical radius for soft-magnetic fine-particles* accepted for publication in *J. Appl. Phys.* in Feb. 2005

[5] **A. Kákay**, M.W. Gutowski, L. Takacs, V. Franco and L.K. Varga, *Langevin granulometry of particle size distribution*, 2004 *J. Phys. A.: Math. Gen.* **37** 6027-6041.