

Influence of space discretization size in 3D micromagnetic modeling

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Abstract

To improve the magnetic properties of ferromagnetic materials, one needs to qualify relations between the microscopic material properties and the macroscopic magnetic behavior. Large computer resources nowadays should make it possible to do this using micromagnetic simulations for larger, bulk like samples. Here, the size of the sample is limited by computer resource restrictions on the number of spatial discretizations in the sample. Generally, the exchange length is seen as the maximum discretization size in micromagnetic computations. This paper shows that in the research area where relations between microstructure and macroscopic magnetic behavior are investigated, larger discretization sizes can be used. This is demonstrated using a micromagnetic hysteresis model.
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1. Introduction

The micromagnetic theory is successfully used in the simulation of storage media. Here, the magnetic dynamics in storage entities is studied in order to ensure fast writing processes e.g. Ref. [1], interactions between different magnetic data spots in patterned media e.g. Ref. [2], etc. Most of the studied samples are ferromagnetic thin films or uniaxial ferromagnetic entities like nanodots. However, the large computer resources nowadays open new application opportunities for the micromagnetic theory. Indeed, the magnetic dynamics in electrical steels used in machine cores and transformers is based on the same interactions as described by the micromagnetic theory. Hence, the micromagnetic theory can be used in the research area of electrical steels, where microstructural material parameters are sought that minimize the iron losses in ferromagnetic materials used in electromagnetic devices, resulting in a lower energy consumption. Using the micromagnetic theory, the description of the magnetic behavior of the material starts from microstructural features like grains, textures, stresses, crystal defects, etc.

The samples simulated in the storage entities research differ vastly from these studied in the research for optimal electrical steel. First, the storage entity samples have a well-known microscopic texture without any lattice defects. In contrary, the electrical steel samples consist of numerous grains of which only a distribution of lattice orientations is known. They contain all kinds of lattice defects: edge and screw dislocations, interstitials, microcracks, etc. The exact locations of these defects is not known, only a defect density and statistical spreading can be assumed. Second, the dimensions of the studied samples differ a lot. The storage entities have dimensions in the order of 10 to 100 nm, while the electrical steel samples are much larger, bulk like. The size of the simulated electrical steel samples is limited by the memory resources available and is determined by the discretization size used to describe the magnetization dynamics in the material.

2. The micromagnetic hysteresis model

A 3D micromagnetic model has been constructed to evaluate the magnetic behavior of electrical steel samples [3]. The samples are discretized using cubic finite difference (FD) cells with edges of length Δ . In the cells the

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magnetization is assumed homogeneous and is represented by a magnetic dipole in the center of the FD cell. According to the micromagnetic theory, the amplitude of each magnetic dipole is fixed, but the orientation varies in space and time.

In the bulk like samples considered here, many vortex states and domain walls can be formed since the number of metastable states is extremely high. Hence, the applied field is assumed to change quasi statically to ensure that the system is always in static micromagnetic equilibrium. Therefore, the external applied field \mathbf{H}_a is discretized on a macroscopic time scale of the order of ms and approximated with a piecewise constant time function. It is assumed that at the moment the applied field jumps from one constant value to the next one, the system is in micromagnetic static equilibrium. The new equilibrium state corresponding with the next value of the applied field is determined by time stepping the Landau–Lifshitz equation (LL equation) in each FD cell until the next micromagnetic static equilibrium state is reached [3]. Here, a microscopic time step δt of the order of ps is used. Time stepping the LL-equation ensures that a next equilibrium state is reached for which the total free energy of the system is an ever decreasing function of time during evolution to that state. Once the equilibrium is reached, the applied field takes a next jump and the next magnetization state is computed, etc.

This numerical scheme differs from the schemes used in the storage entities research where generally only the equilibrium states corresponding with a digital 0 and a digital 1 are important and the switching process between the equilibrium states is much more important than in the micromagnetic hysteresis model described here. In the storage entities research, efficient implicit time stepping schemes for the LL-equation are developed, e.g. Ref. [4]. They allow large microscopic time steps δt , but demand solving a large system of globally coupled nonlinear equations every time step, which is not feasible for the large number of FD cells in the bulk like samples. The large number of FD cells obliges the use of explicit methods in the micromagnetic hysteresis model the predictor-corrector semianalytical time integration scheme [5] for the LL-equation is used. It is an explicit time stepping method allowing relatively large time steps δt . It also preserves the amplitude of the magnetic dipoles and ensures the decrease of the total free energy during the evolution to equilibrium states. The most time consuming part in this (and other) time stepping schemes is the evaluation of the magnetostatic field, using FFT's, during each time step which scales $\mathcal{O}(N \log N)$, with N the total number of FD cell [3].

3. Spatial discretization size

The use of a smaller discretization size Δ not only drastically increases the number of FD cells N for a given sample, it has also a large impact on the microscopic time

step δt needed in the time stepping scheme. Indeed, when smaller FD cells are used, smaller microscopic time steps δt have to be used in the predictor-corrector semianalytical time stepping scheme to guarantee convergence between two successive equilibrium magnetization states. In Ref. [5] it is demonstrated that when Δ is decreased with a decade, the maximum δt for which the system converges decreases by roughly two decades. Hence, the use of smaller FD cells not only leads to more FD cells, but moreover the time stepping of the LL-equation in all these FD cells has to be performed with smaller time steps δt , leading to an increasing number of time steps.

For a given sample, the CPU time needed to simulate the hysteresis loop is dramatically reduced when larger discretization sizes Δ are used. However, in the storage entities research area, the exchange length is seen as the maximum discretization size because on a smaller scale no inhomogeneities can take place [6]. In the electrical steel samples (iron) the exchange length is about 2.8 nm. To examine if the exchange length is also an upper bound in the micromagnetic hysteresis model for electrical steels, hysteresis loops are simulated for an iron sample with dimensions of $0.32 \mu\text{m} \times 1.28 \mu\text{m} \times 0.32 \mu\text{m}$ using different discretization sizes. The external field is applied along the longest edge of the sample. A discretization size of 2.5 nm (slightly smaller than the exchange length), 5.0 nm and 10 nm is considered. The hysteresis loops are shown in Fig. 1.

The loops are very similar: they have the same slope and enclose a similar surface, two important aspects of electrical steels for their performance in electromagnetic devices. Table 1 shows the simulation data for the loops of

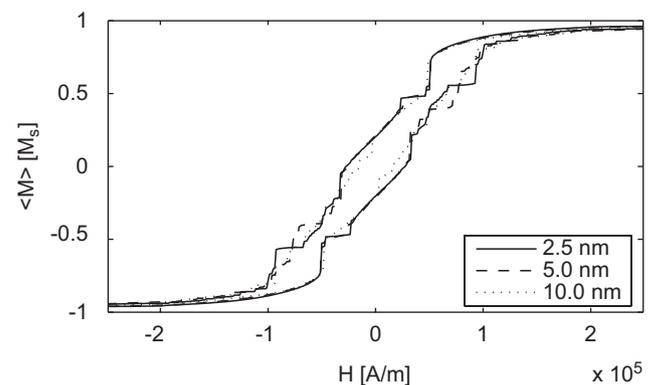


Fig. 1. Hysteresis loops of an iron sample using different discretization sizes Δ .

Table 1
Simulation data for the simulated loops of Fig. 1

Δ (nm)	N	δt (ps)	$\#\delta t$	CPU time
2.5	8 388 608	0.5	27 036	103 h 15 min
5.0	1 048 576	1.0	14 627	8 h 33 min
10	131 072	5.0	1163	7 min 46 s

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