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Micromagnetic investigation of reversal processes in SmCo/Fe exchange-coupled magnets

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Abstract

The main aim of the present investigation is to develop a technique of 3D computer simulation of SmCo/Fe bilayer exchange-coupled magnets composed of hard and soft magnetic layers. These materials are of great interest now because of the very high values of maximum energy products observed in them; at the same time their computer simulation is rather difficult due to several physical and computational reasons. In present report we review some of these difficulties and propose a technique that may help to go round them.
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1. Introduction

Bilayer exchange-coupled magnets (BECM) are composed of a soft magnetic layer that is exchange-coupled to a magnetically hard layer. The soft layer provides high magnetic moment while the hard layer (usually rare-earths-based) provides high anisotropy and coercive fields. Such composite magnets are characterized by extremely large values of maximum energy density product, thus being promising for various applications like new permanent magnets. They are under extensive studies nowadays and computer simulation is one broadly used technique in this field.

Some useful results in BECM simulation one may obtain using simple one-dimensional (1D) model [1]. In the frame of this model, bilayer is divided into a set of layers several angstroms thick and each layer is considered to be a sole spin. For the case of enough thick soft layer, experimental

hysteresis loops for SmCo/Fe bilayers were well fitted using this model. With its help, the maximum energy density products of different bilayers were calculated. It was revealed that the highest values of this parameter are expected for bilayers which are composed of Fe and SmCo layers each less than 50 Å in thickness. However, for these thicknesses 1D model overestimates the switching fields. In this case, full 3D investigation is required to provide good description of the system.

Our main objective was to develop an accurate 3D simulation technique. The investigation is focused on the case of ultra-thin layer thicknesses. As it shows, the value of switching field of a finite (sub-micron) sample with randomly distributed defects depends strongly on a particular defect distribution. Simulation of samples with larger area requires rather huge computational resources (see below the details) and seems to be too expensive in terms of CPU time. A technique that may help to go round these difficulties is proposed here.

The case of thick enough (e.g. 20 nm) layers may be fitted using 1D model disregarding defects, as it was shown in

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Ref. [1]. The case of intermediate layers (about 10 nm thick) was treated by Schrefl et al. [2] using full 3D finite-element technique. In this work good qualitative agreement of the obtained demagnetizing curves with experiment was obtained, that allowed estimation of the maximum energy products; unfortunately no information about the dependence of switching parameters on the defect distribution was presented.

In our case the reversal processes were studied with help of our home-made micromagnetic package SpinPM, using integration of Landau–Lifshitz–Gilbert (LLG) equations and rectangular computational grid, see details of the technique in Ref. [3]. Simulations were performed for the case of zero temperature.

2. SmCo monolayer films

2.1. Role of defects

Most obviously the 1D model fails when one tries to describe hard monolayers in its frame. According to simple theory predictions, the switching field H_s at zero temperatures obeys $H_s = 2K/M_s$, K is anisotropy constant of the film and M_s is the saturation magnetization. For SmCo films ($K = 5 \times 10^7$ erg/cm^3, $M_s = 550$ emu/cm^3 [1]) that yields switching field $H_s^{th} = 18.2$ T against the coercitive field of 7.3 T at 25 K observed in experiment [1]. (As hysteresis loops for SmCo layers and for SmCo/Fe bilayers with ultrathin soft layers are very close to square, the difference between coercitive field, switching field and nucleation field of the film is disregarded here and further).

Computer simulation of homogeneous SmCo monolayers of different sizes with the given parameters yields very close to H_s^{th} values of switching field (e.g. 18.20, 18.26 and 18.68 T for rectangular films 1 nm thick $1 \times 1 \mu^2$, $0.2 \times 0.2 \mu^2$, 50×50 nm^2 in size correspondingly), thus edge effects should not be responsible for the disagreement with the experiment. The main reason of this disagreement lies in inhomogeneity of internal properties of SmCo films. Films have granular structure and the difference of microstructural features of grains causes domain wall (DW) formation and magnetization reversal at lower fields. Thus to provide description of ECM, granular structure of the films should be considered.

2.2. Defects in SmCo films

High-resolution electron tunnel microscopy of investigated in [1] SmCo films (SmCo ($1\bar{1}00$) on MgO(110) substrate with Cr(211) buffer layer [4]) revealed granular structure. Grains were in average 50 nm in size and contained mixture of different compounds (SmCo$_3$, Sm$_2$Co$_7$, SmCo$_5$) of the common prototype. That results in the difference of anisotropy energy K, saturation magnetization M_s in different grains. Magneto-optical investigation of SmCo/Fe bilayers performed in Ref. [5] gives evidence that anisotropy axes of microdomains may

deviate appreciably from an average position (an estimation of average angle of easy axis deflection gives about 20°).

We performed simulation of rectangular nanocristalline SmCo films. Granular structure was randomly generated in a film for various film shapes and sizes (from 50×50 nm^2 up to $1 \times 1 \mu^2$) and grain sizes distributions (with average size ranging from 8 to 55 nm). As a random parameter of individual grain deviation of uniaxial anisotropy axis was chosen in our investigation; the rest of parameters were kept constant. Short investigation showed that the choice of uniaxial anisotropy constant K or magnetization of saturation M_s as a random parameter of a grain leads to very similar peculiarities in the reversal processes. The details of this investigation will be published elsewhere.

On applying external field on a sample previously magnetized until saturation in opposite direction, magnetization in grains starts to rotate in different directions (see Fig. 1(a)). Any of the grains in which magnetization is deflected on appreciable angle (say several tens of degrees) with respect to surrounding grains, constitutes a domain wall nucleus (DWN), i.e. domain boundary located on the border of a grain. The value of external field H_{nucl} at which a DWN transforms into domain walls strongly depends on the surrounding grains features. At some critical field a
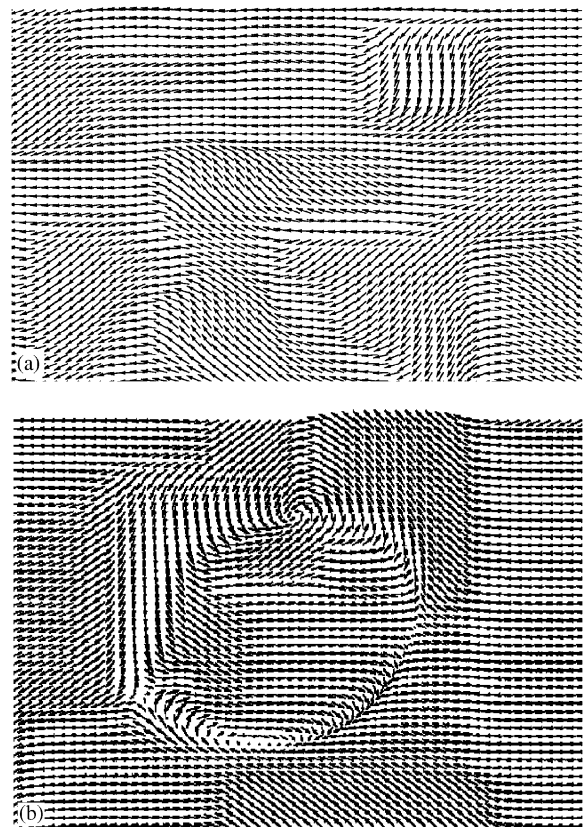

Fig. 1. (a) Magnetization distribution in a fragment of a SmCo film with randomly generated grains at external field 9.0 T (each array represents magnetization averaged over four cells). (b) Expanding (in time) DW transformed from a DWN.