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Do micromagnetic simulations correctly predict hard magnetic hysteresis properties?

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ABSTRACT

Micromagnetic calculations using the finite element technique describe semi-quantitatively the coercivity of novel rare earth permanent magnets in dependence on grain size, grain shape, grain alignment and composition of grain boundaries and grain boundary junctions and allow the quantitative prediction of magnetic hysteretic properties of rare earth free magnets based on densely packed elongated Fe and Co nanoparticles, which depend on crystal anisotropy, aspect ratio and packing density. The nucleation of reversed domains preferentially takes place at grain boundary junctions in granular sintered and melt-spun magnets independently on the grain size. The microstructure and the nanocompostion of the intergranular regions are inhomogeneous and too complex in order to make an exact model for micromagnetic simulations and to allow a quantitative prediction. The incoherent magnetization reversal processes near the end surfaces reduce and determine the coercive field values of Co- and Fe-based nanoparticles.

1. Introduction

The search for candidates of suitable magnetic materials, structures and their expected behavior as reduction of the heavy rare earth content or the replacement for rare earth containing permanent magnets is of great economical and scientific interest [1–4]. Micromagnetic simulations have been widely used for the interpretation and visualization of experimental results. In addition, the aim should be the prediction of the limits of the hard magnetic hysteretic properties, switching time and reversal mechanisms of new materials which will be verified by experiments [5–7]. In this paper we will show that a combination of electronic structure calculations of the intrinsic magnetic properties together with finite element micromagnetic simulations based on the Landau–Lifshitz–Gilbert equation [8] for magnetization reversal is a successful method to describe the influence of the real microstructure on the hysteresis properties of large grained sintered and small grained melt spun rare earth magnets. The micromagnetic model will be extracted from high resolution, nanoanalytical TEM investigations of various RE–Fe–B sintered magnets with different RE contents and coercive field, respectively. The aim of the numerical simulations is to clarify the role of heavy rare earth elements (Dy,Tb) on the coercive field of the magnet and to understand the inhomogeneity of composition and structure near grain boundaries and the influence on local variations of the saturation polarization J_s and the magnetocrystalline anisotropy K_1 on the coercive field H_c.

We also have performed numerical finite element micromagnetic simulations in order to study the possibility of shape anisotropy effects of packed Fe and Co based nanorod structures as candidates for rare earth free permanent magnetic applications and to calculate the coercive field, remanence and energy density product depending on the rod diameter and aspect ratio. Recent developments in nanoscience enabled the production of the nanostructured systems with dimensions approaching the order of few nanometers [9,10].

2. Experimental and micromagnetic simulation procedure

Microstructural and nanoanalytical studies were carried out on an analytical high resolution transmission electron microscope (TEM) (FEI Tecnai F20) at 200 kV equipped with a tungsten field emission gun, a silicon drift energy dispersive X-ray detector, a Gatan Tridem GIF electron energy loss spectrometer (EELS) and a high angle annular dark field detector (HAADF). Thin foil specimens for the nanoanalytical TEM investigation were prepared using the lift-out technique in a focused ion beam (FIB) (FEI Quanta 200 3D DBFIB).

Micromagnetic simulations have been carried out with the FEMME software package, a hybrid finite element/boundary element method (FEM/BEM) code [11]. FEMME solves the Landau–

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Lifshitz–Gilbert equation on a finite element discretization of the magnetic volume. The input parameters are the uniaxial magnetocrystalline anisotropy constant K_1 (K_1 and K_2 for cubic cases), the saturation polarization J_s. and the exchange stiffness A. The easy axis can be rotated with a polar angle θ and an azimuthal angle φ. Paramagnetic materials (grain boundaries) can be simulated by setting magnetocrystalline anisotropy and exchange stiffness to zero. Non-magnetic materials (weak dia- or paramagnets) have additionally a small but non-zero saturation polarization or are not part of the finite element mesh.

The calculation of the demagnetizing field H_{mag} is the computationally most intensive part of the simulation. Only for special geometries (rotational ellipsoids) it is possible to give an exact analytical solution. The demagnetizing field acts as an additional nucleation mechanism but it is also responsible for the shape anisotropy increasing coercivity. Simulations results without demagnetizing field are marked with H_{mag}=OFF throughout this paper. The coercivity of these simulations is only based on exchange and magnetocrystalline anisotropy. Comparing results with H_{mag}=OFF and H_{mag}=ON makes it possible to quantify the influence of the demagnetizing field.

3. Results

3.1. Sintered Nd–Fe–B magnets

Nanoanalytical TEM investigations were carried out to determine the morphology and chemical composition of the several phases occurring in sintered Nd–Fe–B permanent magnets. Sample (a) is free of heavy rare earths (HRE), like dysprosium and terbium, and was produced with He jet milling in order to obtain the smallest possible grain size of 1.4 μm ($\mu_0 H_{cJ} \approx 2.1$ T). Sample (b) has 2.4 wt% of Tb in its starting composition and the standard milling gas nitrogen was used resulting in an average grain size of 3.4 μm ($\mu_0 H_{cJ} \approx 3.0$ T). Fig. 1 shows two TEM specimens produced

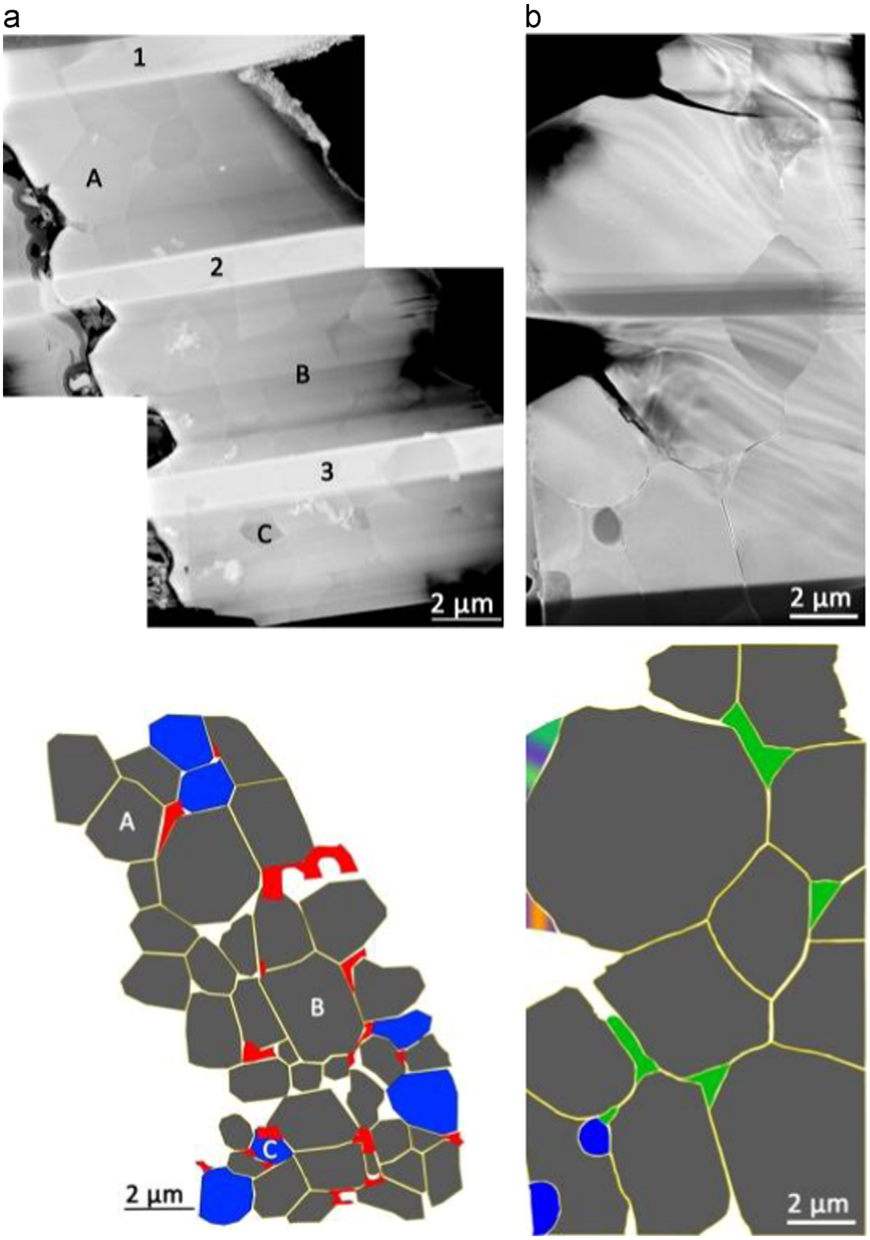

Fig. 1. TEM image of a FIB lamella of a HRE-free sintered Nd–Fe–B magnet (a) and of a sintered (Nd,Tb)–Fe–B magnet (b). The lower two images show the morphology of the samples where the phases are colored. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)