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# Micromagnetic analysis of spin-reorientation transitions. The role of magnetic domain structure



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#### ABSTRACT

A method for calculating micromagnetic state of ferro- or ferrimagnetic single-crystals based on the Néel's method of phases is proposed. The standard Néel technique requires different approaches to calculation of micromagnetic state of samples with different anisotropy types. Furthermore, this technique cannot be used to calculate magnetization curves of materials with a complex anisotropy type, in which the first-order magnetization process (FOMP) occurs. On the contrary, the technique proposed in the present work makes it possible to calculate micromagnetic state of a sample within one unified approach. This technique has no limitations in terms of the anisotropy type as well. In case of the FOMP, the simulation methods that we used show results different from conventional calculation in single domain particle (so-called Stoner–Wohlfarth model). We explain this discrepancy by the fact that a magnetiz domain structure appears in the region of the FOMP. In the present work we show that magnetization processes do not occur in a jump under the FOMP but gradually pass though nucleation and new high-field phase growing, which substitutes for the low-field phase.

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#### 1. Introduction

Magnetic anisotropy constants  $K_{I}$ , $K_{2}$ ,... $K_{n}$  of a ferro- or ferrimagnet can be found from experimental magnetization curve  $I_{exp}$  (H) measured along various crystallographic directions. This method is based on the approximation of  $I_{exp}(H)$  by a calculated dependence  $I_{calc}(H,I_{s},K_{1},K_{2},...K_{n})$ , where  $K_{1}$ , $K_{2}$ ,... $K_{n}$  are fit parameters. The  $K_{1}$ , $K_{2}$ ,... $K_{n}$  values, which provide the best fit, are considered to be experimentally obtained anisotropy constants. From this point of view, it is very important to use a relevant model reflecting real magnetization processes for  $I_{calc}(H,I_{s},K_{1},K_{2},...K_{n})$ .

The commonly used methods of calculating  $I_{calc}(H,I_s,K_1,K_2,...K_n)$  are based on the Stoner–Wohlfarth model [1]. These methods imply a coherent magnetization rotation in a single domain particle. In this case  $I_{calc}(H,I_s,K_1,K_2,...K_n)$  is simulated by the rotation of

*E-mail addresses:* skokov\_k\_p@mail.ru (K.P. Skokov), yupast@mail.ru (Y.G. Pastushenkov), tsv@csu.ru (S.V. Taskaev), valeriarodionova@gmail.com (V.V. Rodionova). spontaneous magnetization  $I_s$  under the applied external magnetic field H [1,2]. As we imply that the sample is in single-domain state, the magnetization value I is the projection of  $I_s$  onto the direction of the external magnetic field H. The angle between the external field H and the vector  $I_s$  can be found by minimizing the total energy, which consists of the anisotropy energy and the energy of a magnetic moment in an external magnetic field. The advantage of this technique is its simplicity.

On the contrary, the Néel's method of  $I_{calc}(H,I_s,K_1,K_2,...K_n)$  simulation is based on the assumption that a sample can be subdivided into magnetic domains in low magnetic fields. Thus, the total energy should include the demagnetizing field energy of a specimen, the anisotropy energy and the magnetic moment energy in the external magnetic field. In this case, all the domains contribute to the projection of the net magnetization onto the external field direction. The advantage of the Néel's method is that it gives a more detailed description of magnetization processes [3–5].

In this work we show that both simulation methods lead to identical magnetization curves for the 'regular' anisotropy types, such as 'easy axis,' 'easy cone,' and 'easy plane.' However, in the event of an additional metastable minimum of anisotropy energy,





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which, in turn, shows up as the first order magnetization process (FOMP), these simulation methods show different results. We explain this discrepancy by the fact that a magnetic domain-like structure appears in the region of the FOMP-transition.

#### 2. Methods

During the study of the first order magnetization process (FOMP), the method for calculating magnetization curves with the assumption that the sample is in a single-domain state is typically used for analyzing the results of magnetic measurements. In this case, magnetization vector projection on the coordinate axes can be written as:

$$I_{x} = I_{s} \cdot \sin(\phi) \cdot \cos(\theta)$$

$$I_{y} = I_{s} \cdot \sin(\phi) \cdot \sin(\theta)$$

$$I_{z} = I_{s} \cdot \cos(\phi)$$
(1)

where angle  $\phi$  is the angle between the magnetization vector and c axis of the crystal and angle  $\theta$  is the angle between vector  $\vec{l_s}$  and plane *xOz* (see Fig. 1a). Taking into account the anisotropy energy (the present work uses a tetragonal magnetic as the example) and the energy in the external magnetic field only, the crystal energy density can be written as

$$E(\phi, \theta) = K_{1} \cdot \sin^{2}(\phi) + K_{2} \cdot \sin^{4}(\phi) + K_{3} \cdot \sin^{4}(\phi)$$
$$\cdot \cos(4\theta) - \dots$$
$$\dots - I_{s} \cdot H \cdot (\sin(\phi) \cdot \cos(\theta) \cdot \sin(\Phi) \cdot \cos(\theta) + \sin(\phi) \cdot \sin(\theta)$$
$$\cdot \sin(\Phi) \cdot \sin(\theta) + \cos(\phi) \cdot \cos(\Phi))$$
(2)

where  $\Theta$  and  $\Phi$  are polar and azimuthal angles defining the external magnetic field direction in relation to the coordinate axes (see Fig. 1a);  $K_1$ ,  $K_2$ , and  $K_3$  are anisotropy constants; and  $I_S$  is the saturation magnetization. To find the magnetization projection using expression (1), we need to find such values for  $\phi$  and  $\theta$  when  $E(\phi, \theta)$  is minimal.

This approach was suggested by Asti to analyze field-induced FOMP phase transitions [2] (in the event of two dimensions). On one hand, this method does not take into account the presence of a domain structure in a sample. On the other hand, taking into account the influence of domain structure transformations in an external field on magnetization reversal processes can provide additional information on the material's characteristics in the event of magnetic phase transitions.

To calculate the micro-magnetic state of ferro- and ferrimagnetic single crystals, the present work uses the method based on the Néel's theory of phases [3–5], taking into account the specimen's domain structure. Unlike the standard Néel's method, which requires different approaches to calculating micromagnetic state of a sample for different anisotropy types and is not applicable to calculating magnetization curves for a ferromagnetic with a complex anisotropy type ('easy plane+metastable easy axis' or 'easy axis+metastable easy plane'), the method suggested in the present work allows us to calculate the micromagnetic state of a sample for any type of the magnetic anisotropy.

The Néel's method is based on the following assumptions:

- In the absence of a magnetic field, the sample is broken down into magnetic domains. The domains with the same direction of magnetization (or domains of the same sign) comprise a "phase." In the external field magnetization occurs due to the magnetization vector rotation as well as due to the domain wall motion.
- 2. When the value and/or direction of the magnetic field are changed, the volumetric densities of the energy of different domains change as well. Due to both magnetization processes the rotations and domain wall motions—the magnetic domains configuration starts changing in order to reach equal energy densities of different "phases." The influence of domain walls is neglected.
- 3. The volumetric density of the sample's energy is comprised of the volumetric energy densities of anisotropy  $E_{A_1}$  the energy in the external field  $E_{H_1}$  and the energy of the demagnetization



**Fig. 1.** Magnetization and external magnetic field for both models (a) Stoner–Wohlfarth; (b) Néel's model. The case of uniaxial magnetic anisotropy.  $\phi$  is the angle between the magnetization vector and *c* axis of the crystal; angle  $\theta$  is the angle between vector  $\vec{l}_s$  and plane *xOz*.  $\Theta$ ; and  $\phi$  are polar and azimuthal angles defining the direction of the external magnetic field.

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