Journal of Magnetism and Magnetic Materials 330 (2013) 81–87

Contents lists available at SciVerse ScienceDirect

Journal of Magnetism and Magnetic Materials

journal homepage: www.elsevier.com/locate/jmmm

Effective elastic and magnetoelastic anisotropies for thin films with hexagonal and cubic crystal structures

Vagner Z.C. Paes, Dante H. Mosca *

Departamento de Física, Universidade Federal do Paraná, C.P. 19044, 81531-990 Curitiba-PR, Brazil

ARTICLE INFO

Article history:
Received 11 September 2012
Received in revised form
16 October 2012
Available online 1 November 2012

Keywords:
Anisotropy
Thin film
Magnetoelastic

ABSTRACT

In this work we present a detailed study on the elastic and magnetoelastic contributions for thin films and bulk materials with hexagonal and cubic crystalline structures. In contrast to bulk materials, the effective elastic anisotropy for thin films shows a strong dependence on the epitaxial order of the film on the substrate and the stress-free condition of the out-of-plane strain. The contributions of the elastic and magnetoelastic energies in the effective magnetic anisotropy of films with cubic or hexagonal lattice are obtained for certain epitaxial growth directions.

1. Introduction

Ferromagnetic materials are intrinsically magnetostrictive, developing a mechanical deformation when subjected to an external magnetic field (see Fig. 1). This phenomenon comes from a reorientation of the magnetization direction in the material exposed to a magnetic field, leading to a field-induced strain. In a given structure, the atoms are in an equilibrium position and the elastic energy is responsible for a stable equilibrium of atomistic positions with magnetization assuming a preferential direction.

In ferromagnetic thin films have been reported that elastic and magnetoelastic contributions differ substantially from the respective bulk properties [1]. Magnitude and sign of magnetoelastic coupling constants can deviate from their respective bulk value mainly in the case of ultrathin and strained ferromagnetic films. The preferential magnetization orientation can also be influenced by the lattice deformation. Since first-order magnetoelastic effects in strain are well-known for several crystalline structures [2,3], elastic constants, magnetoelastic couplings and strains are appropriate parameters to model the influence of stress in the magnetization process.

Even today, an accurate numerical solution for three- and two-dimensional elastostatics and magneto-elastostatic of films is often impractical and sometime infeasible. Magneto-elastic displacements depend on the spin–orbit interaction and can locally differ from the rigid body displacements, making necessary use of the finite strain tensors with compatibility conditions to leave the body without unphysical gaps or overlaps after a deformation. Therefore, both first-principles calculations and finite element methods become complicated approximations for our purpose of analyses, it is sufficient to apply appropriate boundary conditions to differentiate bulk and thin films. For our purpose of analyses, it is sufficient to apply appropriate boundary conditions to differentiate bulk and thin films. Whereas bulk is free to deform in all directions, thin films are considered homogeneous and linearly elastic slabs bounded by two flat faces, one is free to deform and the other is clamped on a substrate.

Elastic and magnetoelastic effects are treated assuming that free energy should be expressed as a function of the external magnetic field and temperature so that the derivative with respect to magnetic field gives the magnetization at constant temperature. In these procedures, is admitted that volume and number of magnetic moments are constants.

In the early work of Kittel [2,4–7] it was shown that the effect of a tetragonal deformation in cubic bulk materials leads to a correction in the free magnetic energy density. In general, first- and second-order magnetoelastic terms, i.e., terms that scale to α_i^2 and α_i^4, are used in the free magnetic energy to describe the magnetic behavior of thin films [3,4,8–13]. The origin of these terms, however, remains unclear. The current work provides expressions for those terms depending on the epitaxial order, showing that magnetoelastic effects in thin films are a very complicated issue and their effects in the magnetic anisotropy are captious.

In this work we analyze the effects of unit cell distortion in the magnetic anisotropy as thin films are constrained to the substrate. In this case, additional non-linear terms are obtained in the

* Corresponding author. Tel.: +55 41 3361 3405; fax: +55 41 3361 3418.
E-mail addresses: vzeizer@gmail.com (V.Z.C. Paes), mosca@fisica.ufpr.br (D.H. Mosca).

0304-8853/$ - see front matter © 2012 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.jmmm.2012.10.036

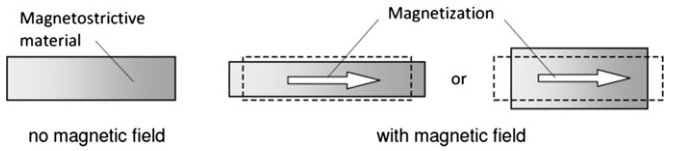

Fig. 1. Magnetomechanical behavior of a magnetostrictive material, which can be stretched (left part) or shrinked (right part) under an applied field.

total magnetic anisotropy, leading to elastic free energy density for thin-films substantially different from those obtained for bulk. Moreover, such magnetic anisotropy constants depend strongly on the epitaxial relation of the film on the substrate.

2. Magnetoelastic and elastic contributions

Magnetoelastic energy and its corresponding magnetoelastic coupling constant take into account the interaction between the magnetization and lattice deformation due to strain [2]. The magnetoelastic energy is defined zero for an unstrained lattice. Magnetostrictive energy is due to deformation of a sample due to magnetic interactions and can be spontaneous when originated from internal magnetic interaction or forced when created by magnetic interaction between the sample and an externally applied magnetic field. Consequently, magnetic and elastic properties in ferromagnetic materials depend on each other and there is a strong influence of crystalline structure and lattice deformation in the magnetization process and elastic properties.

The application of a mechanical stress to magnetic material changes its magnetic properties. Such changes are visible in the magnetization curve and make the magnetic induction different for a given magnetic field at different applied stresses. These changes are due mainly to two mechanisms. One is due to the magnetoelastic energy, which modifies the anisotropy of the material and the other is due to a change in the interatomic distances and symmetry lowering.

In most of the models of magnetostriction and magnetoelastic coupling, the energy is separated into magnetic energy and elastic energy, with the sum of which is considered as the magnetoelastic energy of the coupled system.

In bulk, it is commonly assumed that magnetoelastic and magnetostrictive coefficients of the magnetic material do not change with strain. However, in thin films these coefficients can be assumed to be linearly dependent on the stress values or strain by considering that Hook's law is valid.

The magnetomechanical effects in magnetic materials are useful phenomena as it is used in actuators, transducers and devices, but this same phenomena becomes parasitic when it is considered source of the noise and vibrations in transformers, inductors and magnetic sensors.

Next, elastic and magnetoelastic energies contributions to free energy for magnetic materials with cubic and hexagonal crystalline structures are revised and further implemented in the treatment of magnetic thin films constrained to substrates.

2.1. Hexagonal crystals

The elastic free energy density for a crystal with hexagonal structure, F_{el}^{H}, is given by [14]

$$F_{el}^{H}=\tfrac{1}{2}c_{11}(\epsilon_1^2+\epsilon_2^2)+c_{12}\epsilon_1\epsilon_2+c_{12}\epsilon_3(\epsilon_1+\epsilon_2)+\tfrac{1}{2}c_{33}\epsilon_3^2+\tfrac{1}{2}c_{44}(\epsilon_4^2+\epsilon_5^2)+\tfrac{1}{4}(c_{11}-c_{12})\epsilon_6^2 \quad (1)$$

and the magnetoelastic free energy density, F_{me}^{H}, is [15]

$$F_{me}^{H}=B_1(\alpha_1^2\epsilon_1+\alpha_2^2\epsilon_2+\alpha_1\alpha_2\epsilon_6)-B_2\alpha_3^2\epsilon_3-B_3\alpha_3^2(\epsilon_1+\epsilon_2)+B_4(\alpha_2\alpha_3\epsilon_4+\alpha_1\alpha_3\epsilon_5). \quad (2)$$

Here α_1, α_2, and α_3 are the direction cosines with respect to the c-axis of the hexagonal lattice, ϵ_i represents the strain in Voigt's notation, c_{ij} and B_i denote the elastic and magnetoelastic coupling constants, respectively. It is noteworthy that in Eqs. (1) and (2) second-order strains have not been taken into account, which might also play a role.

2.2. Cubic crystals

According to Kittel [2,1,3] for a crystal with cubic structure, the elastic, F_{el}^{C}, and the magnetoelastic, F_{me}^{C}, free energy densities are, respectively, given by:

$$F_{el}^{C}=\tfrac{1}{2}c_{11}(\epsilon_1^2+\epsilon_2^2+\epsilon_3^2)+\tfrac{1}{2}c_{44}(\epsilon_4^2+\epsilon_5^2+\epsilon_6^2)+c_{12}(\epsilon_1\epsilon_2+\epsilon_2\epsilon_3+\epsilon_1\epsilon_3), \quad (3)$$

$$F_{me}^{C}=B_1(\alpha_1^2\epsilon_1+\alpha_2^2\epsilon_2+\alpha_3^2\epsilon_3)+B_2(\alpha_1\alpha_2\epsilon_6+\alpha_2\alpha_3\epsilon_4+\alpha_3\alpha_1\epsilon_5). \quad (4)$$

In the above equations we omitted higher-order terms in the strain, which might also play a role.

Next, we discuss how is the procedure to evaluate the effective elastic anisotropy for bulk materials and thin films with cubic and hexagonal crystalline structures. It is properly done regarding the epitaxial relations of the films on the substrates and considering the orthogonal crystal coordinate system in which the elastic constants c_{ij} are well defined.

3. Thin films under constraints

On the contrary to bulk materials, which are free to deform under action of a magnetic external field, thin films are clamped on the substrates. Therefore, ferromagnetic thin films are not free to deform under magnetostrictive forces. A magnetostrictive stress is induced along the substrate plane. As a consequence, the strains belonging to the film plane are fixed, while the out-of-plane strains are free to deform.

A word of caution is that all strains are not constant during the magnetization process. Consequently, they always search for an equilibrium position to minimize the total energy. Let the in-plane strains be ϵ_1, ϵ_2 and ϵ_6, while ϵ_3, ϵ_4 and ϵ_5 are the out-of-plane strains [16]. So, the previous discussion is equivalent to:

(I) $\sigma_i=\partial F/\partial\epsilon_i$, $i=1,2,6$.
(II) $\partial F/\partial\epsilon_i=0$, $i=3,4,5$.

Here F is the total free energy density, ϵ_i is the strain in Voigt's notation and σ_i is the field-induced stress.

To correctly take into account the energy due to lattice distortion, we consider that the in-plane strains are constant while the out-of-plane strain are free to relax and distort the lattice, minimizing the energy, and contributing to the effective anisotropy. In this case, the contributions to the in-plane strains may arise from growth conditions, thermal expansion, and eventually structural phase transition.

It is also noteworthy that the effective elastic anisotropy should be calculated by regarding properly the epitaxial relation of the film on the substrate. It should be properly adjusted to the orthogonal crystal coordinate system in which the elastic constants c_{ij} are well defined [1,17]. The coordinates are already properly adjusted in the case of hexagonal crystals with 0001-orientation and cubic crystals with 100-orientation (both body-centered cubic and face-centered cubic elements). However, it is