Journal of Magnetism and Magnetic Materials 430 (2017) 103–108

Contents lists available at ScienceDirect

Journal of Magnetism and Magnetic Materials

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

On the magnetization process and the associated probability in anisotropic cubic crystals

D.M. Khedr[a,*], Samy H. Aly[b], Reham M. Shabara[b], Sherif Yehia[c]

[a] Department of Basic Science, Modern Academy of Engineering and Technology at Maadi, Cairo, Egypt
[b] Department of Physics, Faculty of Science at Damietta, University of Damietta, Damietta, Egypt
[c] Department of Physics, Faculty of Science at Helwan, University of Helwan, Helwan, Egypt

ARTICLE INFO

Keywords:
Magnetization
Magnetic susceptibility
Magnetic anisotropy

ABSTRACT

We present a theoretical method to calculate specific magnetic properties, e.g. magnetization curves, magnetic susceptibility and probability landscapes along the [100], [110] and [111] crystallographic directions of a crystal of cubic symmetry. The probability landscape displays the evolution of the most probable angular orientation of the magnetization vector, for selected temperatures and magnetic fields. Our method is based on the premises of classical statistical mechanics. The energy density, used in the partition function, is the sum of magnetic anisotropy and Zeeman energies, however no other energies e.g. elastic or magnetoelastic terms are considered in the present work. Model cubic systems of diverse anisotropies are analyzed first, and subsequently material magnetic systems of cubic symmetry; namely iron, nickel and Co_x Fe_{100-x} compounds, are discussed. We highlight a correlation between magnetization curves and the associated probability landscapes. In addition, determination of easiest axes of magnetization, using energy consideration, is done and compared with the results of the present method.

1. Introduction

The magnetic properties of cubic crystals have been extensively studied both theoretically and experimentally by many authors [1–14]. For example, an analysis of the magnetic properties of simple cubic systems has been reported using the Heisenberg theory of ferromagnetism [1,2]. The theory of magnetic anisotropy energy (MAE) in *Fe* and *Ni* was first formulated by Brooks and Fletcher [3,4]. Following Akulov's formula [5], magnetization curves were measured on pure iron and on Fe-Co alloy in the temperature range from room temperature to about 50 $^{\circ}$C below the Curie point [6]. An atomistic theory of the thermal and magnetic properties of metallic cerium, with cubic close-packed structure has been reported [7]. By a second order extension of the Callen and Callen model, an approach to the problem of magnetic anisotropy (MA) has been introduced [8,9]. Other investigations [10–13] elaborated the MAE problem using ab initio calculations obtained within the local-spin density approximation (LSDA) to the density functional theory. Also an ab initio study of the magnetization of prototype complex cubic structures was reported [14]. The magnetic and thermomagnetic properties of Fe, Ni and Co-Fe compound, have been experimentally studied [15–21].

In this paper, we present a method based on the laws of classical statistical mechanics, to calculate specific magnetic properties of model and real magnetic systems of cubic symmetry. In particular, we calculate the magnetization curves, magnetic susceptibility, energy and probability landscapes of model systems of three anisotropy constants of different magnitudes and/or signs. We apply both energy considerations and our analysis of the studied model systems to specific material systems e.g. Fe, Ni and Co_x Fe_{100-x} compounds. This method has been successfully used in calculating magnetic and size-dependent properties of certain ferromagnetic systems [22,23].

2. Theory and computation

We choose our coordinate system such that the saturation magnetization $\boldsymbol{M_s}$ makes an angle θ with the $z-$ axis and the projection of $\boldsymbol{M_s}$, on the $x-y$ plane, makes an angle φ with the x axis, which is taken to be the [100] direction of the cubic crystal. Therefore, the direction cosines of $\boldsymbol{M_s}$ are $\alpha_x = \sin\theta\cos\varphi$, $\alpha_y = \sin\theta\sin\varphi$, $\alpha_z = \cos\theta$. The magnetocrystalline anisotropy energy density E_a can be expressed, in terms of a series expansion of α_x, α_y, α_z as follows [5,9]:

$$E_a = K_0 + K_1(\alpha_x^2\alpha_y^2 + \alpha_y^2\alpha_z^2 + \alpha_x^2\alpha_z^2) + K_2\alpha_x^2\alpha_y^2\alpha_z^2 + K_3(\alpha_x^4\alpha_y^4 + \alpha_y^4\alpha_z^4 + \alpha_x^4\alpha_z^4) + \ldots \quad (1)$$

* Corresponding author.
E-mail address: doaamohammed88@gmail.com (D.M. Khedr).

http://dx.doi.org/10.1016/j.jmmm.2017.01.011
Received 7 August 2016; Received in revised form 27 December 2016
Available online 28 January 2017
0304-8853/

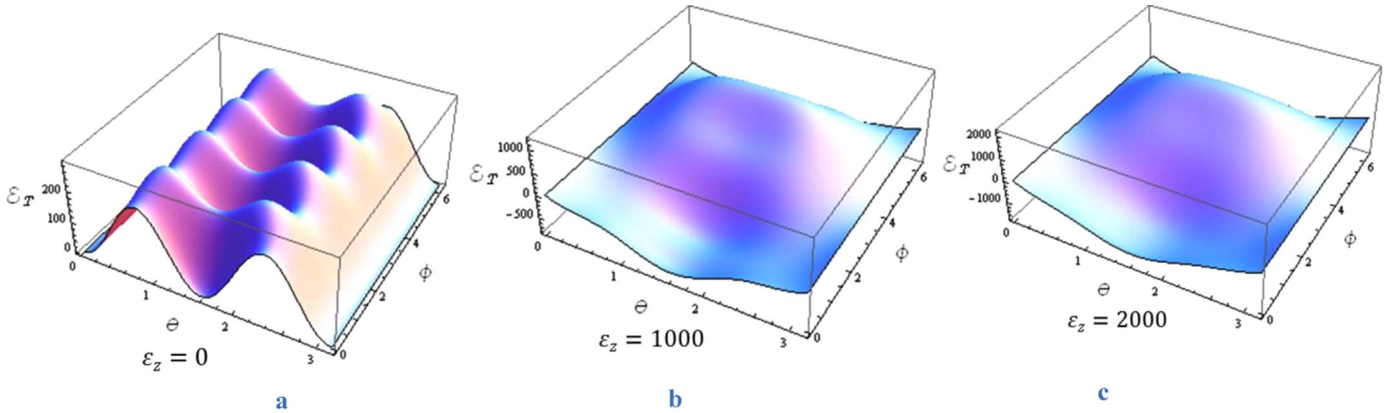

Fig. 1. The change of ε_T with θ and φ for chosen ratio of α : γ : ξ=4 : 2:1 with magnetic field applied along the [110] direction.

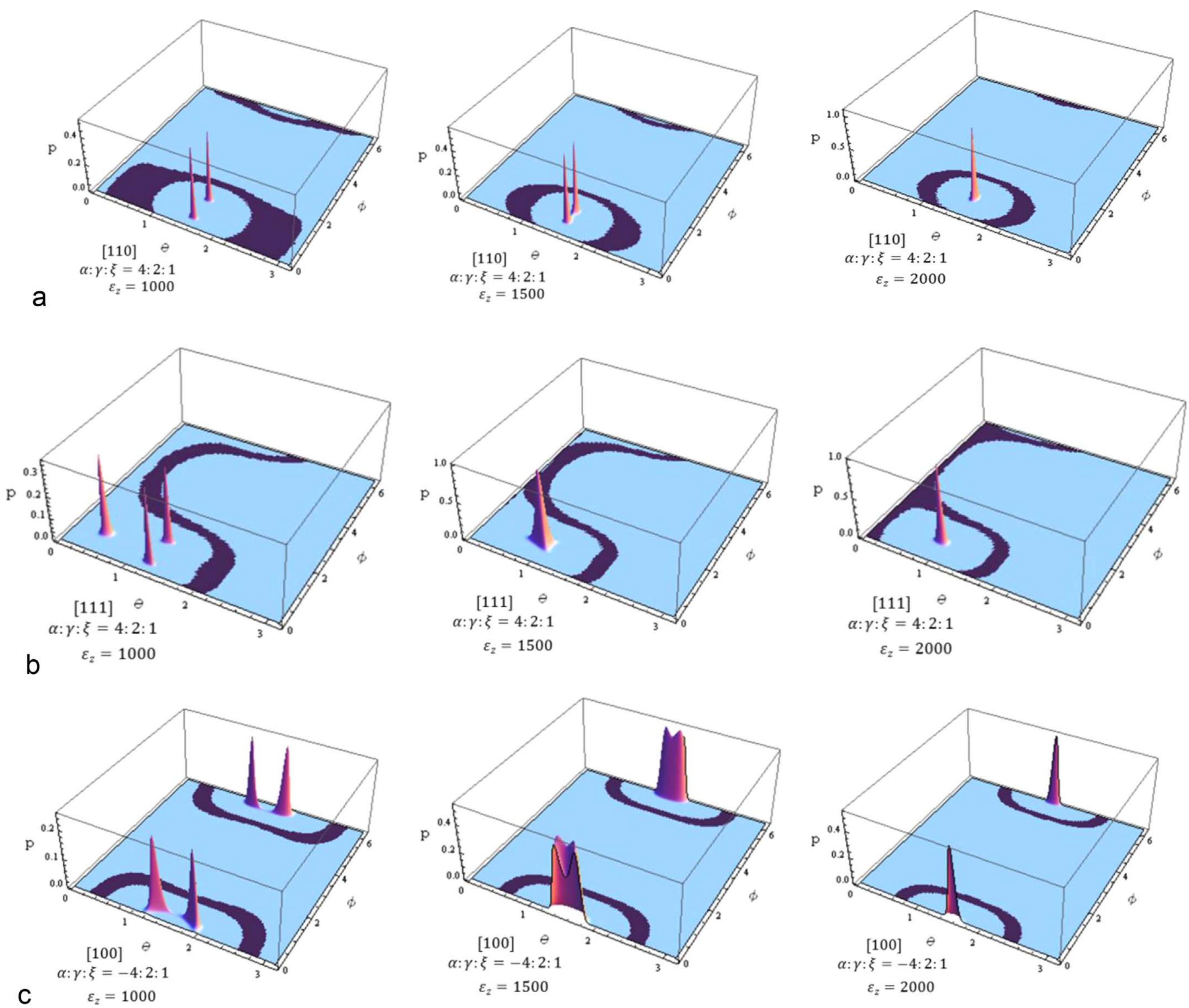

Fig. 2. a: The dependence of the probability landscapes on εz for a system with α : γ : ξ=4 : 2:1, with magnetic field applied along the [110] direction. b: The dependence of the probability landscapes on εz for a system with α : γ : ξ=4 : 2:1, with magnetic field applied along the [111] direction. c: The dependence of the probability landscapes on εz for a system with α : γ : ξ= − 4 : 2:1, with magnetic field applied along [100] direction.

Where K_0, K_1, K_2,. . . are the anisotropy constants, which are usually temperature – dependent. K_0 is independent on angle and is usually ignored. Terms of higher powers are sometimes so small that they may be neglected. Few studies have reported on their magnetic field – dependence e.g. in case of *Fe* [24].

The total energy density E_T is the summation of E_a and Zeeman