

The internal thermal stresses during the cooling process of a nanowire from alumina membrane

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We present in this paper the internal thermal stresses appearing in Co nanowires in alumina template when they are cooled from the room temperature to 3 Kelvin. Thermal stresses are evaluated with a finite element method (FEM), taking into account the difference between the thermal expansion coefficients of cobalt and alumina membrane. The coupling between the magnetostriction and the stress distribution leads to an easy axes distribution associated with a magnetic domain structure consisting of a cylindrical inner core with axial magnetization and a cylindrical outer shell with radial magnetization of about 2% from the entire radius.

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1. Introduction

The magnetic nanowire arrays prepared by electrodeposition in nanopores of alumina membranes form a class of magnetic materials with many technological applications [1]. Consequently, the study of the thermal stresses induced in a nanowire from alumina membrane is receiving a considerable experimental and theoretical attention [2]. During the cooling process in the two materials (nanowire + alumina membrane in contact) radial, azimuthal and axial stresses are induced.

The aim of this paper is the evaluation of thermal stresses during the cooling of Co nanowire from the room temperature $T_w = 300\text{ K}$ to $T_g = 3\text{ K}$ considering both the thermal gradients that appear during the cooling of the nanowire and the different thermal behaviour of the two materials (cobalt nanowire + alumina membrane) in contact. The temperature variation during the cooling process considerably influences the internal stresses in the nanowire. To evaluate the thermal stresses induced during this process we have used finite element method (FEM) distinguishing the following main steps:

(i) The evaluation of the spatio-temporal distribution of the temperature during the forced cooling process. In this case we have analyzed, using FEMLAB/COMSOL package, the spatial and temporal evolution of the temperature in the nanowire-alumina membrane system, considering the thermal boundary conditions at the metal-alumina interface;

(ii) By knowing the spatio-temporal distribution of the temperature in nanowire-alumina system one can obtain the stresses which appear both due to the forced cooling (because of the big thermal gradients) and to constraints produced on the nanowire by the alumina template as a result of the difference between the thermal expansion coefficients of the two materials in contact;

(iii) Discussions about the magnetic domains structure.

2. The temperature in the system

Let's consider an nanowire having the length L , the radius R_1 and thickness of the alumina membrane $g = R_2 - R_1$; where R_2 is the total radius of the cylindrical system (cobalt nanowire + alumina membrane) Fig. 1.

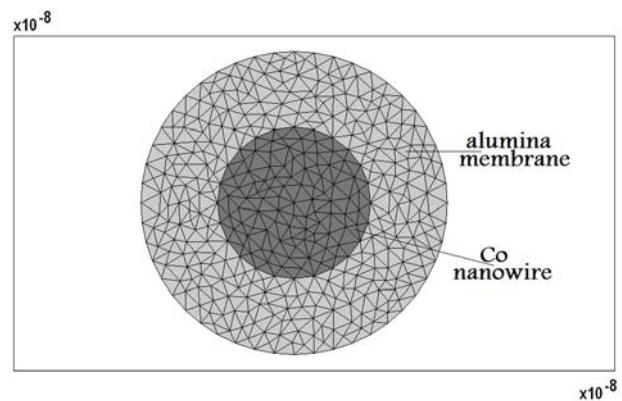


Fig. 1. The cross section of the system (nanowire + alumina).
Geometry discretization.

The evaluation of the thermal stresses induced during the cooling process implies the knowledge of the thermal behavior of the metal-alumina membrane system. The Fourier heat equation for the nanowire [3] is given by:

$$\frac{\partial T_1}{\partial t} = a_1 \left(\frac{\partial^2 T_1}{\partial r^2} + \frac{1}{r} \frac{\partial T_1}{\partial r} \right) - b(T_1 - T_g), \quad (2.1)$$

and

$$\frac{\partial T_2}{\partial t} = a_2 \left(\frac{\partial^2 T_2}{\partial r^2} + \frac{1}{r} \frac{\partial T_2}{\partial r} \right), \quad (2.2)$$

for alumina membrane with the following boundary conditions [4, 5]: (i) the heat flux from the metallic part is received by the alumina cover; This heat flux must be continuous. So, for $r = R_1$ we must have

$$k_1 \left(\frac{\partial T_1}{\partial r} \right) \Big|_{r=R_1} = k_2 \left(\frac{\partial T_2}{\partial r} \right) \Big|_{r=R_1}, \quad (2)$$

where k_1 and k_2 are the coefficients of thermal conductivity of the cobalt and alumina membrane, respectively;

(ii) on the nanowire-alumina interface ($r = R_1$), the temperatures of the adjacent regions must be equal:

$$T_1(r = R_1) = T_2(r = R_1); \quad (3)$$

(iii) the temperature on the outer surface of the system, is equal to the $T_g = 3K$:

$$T_2(r = R_2) = T_g. \quad (4)$$

where $a_1 = k_1 (\rho_{Co} c_{Co} L)^{-1}$, $a_2 = k_2 (\rho_{al} c_{al})^{-1}$, $b = 2k_1 (\rho_{Co} c_{Co} R_1)^{-1}$, ρ_{Co}, ρ_{al} are the mass densities for Co and alumina membrane respectively.

We have calculated the temperature distribution corresponding to system from the Fig.1. Because of the geometric symmetry, the problem was reduced to a bidimensional one, using variables separation method. The equations (1) and (2) were discretized on a domain that contains the system, and taking into account the boundary conditions, a heat transient transfer problem is resulting. The discretization of the surface is realized with triangular elements, the position of the triangle nodes being an input for FEM algorithm. The distribution of the triangular elements is not uniform over the considered domain, the density of elements being higher close to the boundaries. In Fig. 2 one shows the space-time temperature distribution for a system with the nanowire having $R_1 = 5nm$ and the thickness of the alumina cover being $g = 45nm$ ($R_2 = 50nm$). Regarding the time evolution, the temperature decreases from $T_w = 300K$ to the room

temperature $T_g = 3K$, during the time interval of about $t = 0.1 fs$.

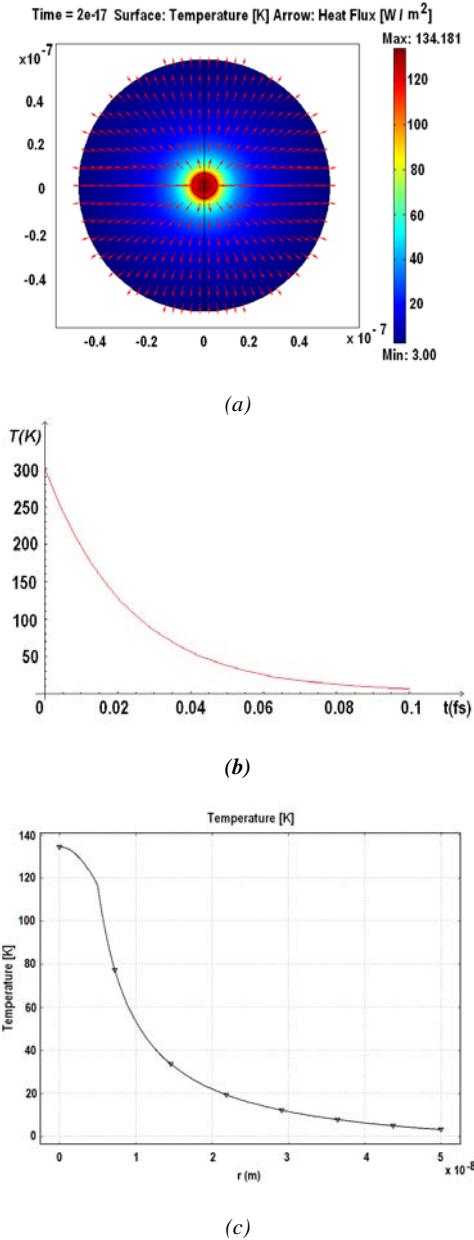


Fig. 2. The thermal behaviour of the system (a) The spatial distribution of the temperature in the cross section of the system; (b) The time evolution of the temperature in the point $r=0$ for the nanowire; (c) The radial distribution of the temperature in the cross section of the system at the moment $t = 0.02 fs$.

3. Internal stresses induced in nanowire

Let's analyze now the spatio-temporal distribution of the stresses which appear both due the thermal gradients

and to the constraints produced on the alumina cover by its cooling, as a result of the difference between the thermal expansion coefficients of the two materials in contact.

In order to obtain the stresses distribution during the cooling process of the system, we have used the spatio-temporal distribution of the temperature presented in the above section.

Using Predefined Multiphysics Coupling Module-Thermal Structural Interaction, for the geometry presented in the Fig. 1, we have imposed the following conditions on the nanowire-membrane interface [6, 7]:

1. the strains that appear in this process result due to the difference between the thermal expansion coefficients of the nanowire and membrane:

$$u_r^{Co}(r = R_1) - u_r^{al}(r = R_1) = \varepsilon R_1;$$

2. the equilibrium condition of the stresses on the nanowire-membrane interface:

$$\sigma_{rr}^{Co}(r = R_1, t) = \sigma_{rr}^{al}(r = R_1, t)$$

3. the equilibrium condition on the exterior surface ($r = R_2$) of the nanowire:

$$\sigma_{rr}^{al}(r = R_2, t) = 0.$$

$$\varepsilon = \varepsilon_{Co} - \varepsilon_{al} = (\alpha_{Co} - \alpha_{al})(T_w - T_g)$$

is the resultant strain; α_{Co}, α_{al} is thermal expansion coefficient for cobalt and alumina respectively;

Using these three conditions we have determined the thermal stresses in the system. In the Fig. 3 are presented the radial stresses induced in the system at the end of the cooling process. The alumina membrane induces the thermal stresses during the cooling of the system. In order to find the magnetic domain structure we must to calculate the stress distribution only for the nanowire. Using the same FEM algorithm, we have calculated the radial, azimuthal and axial stresses for the nanowire when the

system is cooled from room temperature, T_w to T_g (Fig. 4).

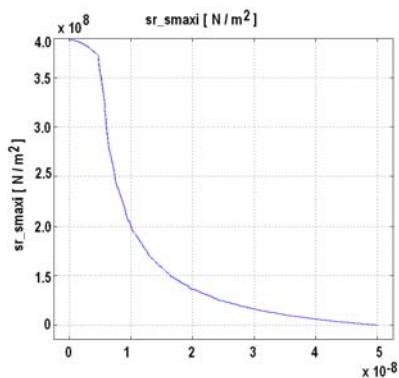


Fig. 3 The radial stresses induced in the system at the end of the cooling process (after $t = 0.1$ fs)

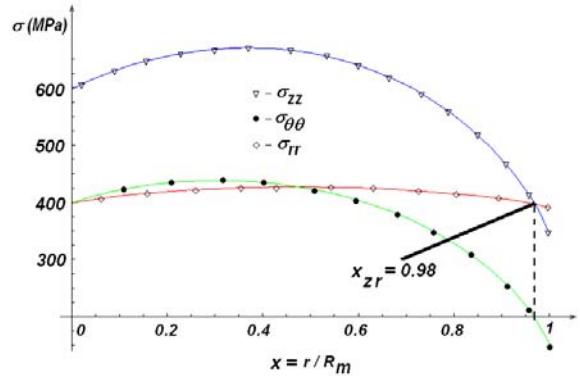


Fig. 4. The radial, azimuthal and axial stresses induced in the nanowire at the end of the cooling process

4. The magnetic domains structure of Co nanowire.

As one can observe from Fig. 4, the stresses distribution leads to a magnetic domains structure of the nanowire as follows: starting from the point $x = 0$ up to the point $x_{zr} = 0.98$ there is a region in which $\sigma_{zz}(x)$ is the component with the highest value and it is positive (zone I). From this point to the point $x = 1$ there is a second region, much narrower than the first one, in which $\sigma_{rr}(x)$ is the highest positive stress component (zone II).

The strong coupling between the internal stresses and the negative magnetostriction of the cobalt determines the appearance in the nanowire of the easy axes of magnetization in the regions in which the dominant internal stresses are tensile (positive). So, the magnetoelastic energy minimization leads to a domain structure with two zones:

- zone I: $x \in [0, x_{zr}]$; due to the coupling between $\sigma_{zz}(x)$ (positive) and the magnetostriction the first zone results, with an uniaxial magnetic anisotropy having the easy axis oriented along the axis of the nanowire (Oz - axis);

- zone II: $x \in (x_{zr}, 1]$; due to the coupling between $\sigma_{rr}(x)$ (positive) and the magnetostriction the second zone results, with a radial magnetic anisotropy. Also, in this zone the compressive component $\sigma_{\theta\theta}(x)$ generates a hard axis of magnetization on the azimuthal direction;

Synthesizing, we can state that the stress distribution from Fig. 4, coupled with the magnetostriction of the Cobalt, leads to an easy axes distribution associated with a domain structure which consist of a cylindrical inner core (IC) with axial magnetization (zone I) and an outer shell (OS) with radial magnetization (zone II).

5. Conclusions

The numerical results described in this paper shows the distribution of the stresses induced in the Co nanowire, during its cooling from the room temperature, to 3 Kelvin temperature.

Using FEMLAB and considering the thermal behavior of the system during the cooling process, we calculated the stresses induced by the alumina membrane, due to the different cooling of the two materials in contact.

In the thermal evolution of the nanowire, the longer the time interval from the beginning of the cooling process, the smaller the difference between the temperature in the center of the nanowire and the temperature on the metal-membrane interface.

The center of the nanowire "reaches" the temperature $T_g = 3K$, in approximately $t = 0.03 fs$ from the moment of the material's cooling.

The three stresses (radial, azimuthal and axial stresses) depend on the radius of the nanowire, being positive. The magnitude order of these stresses is $10^8 Pa$; Concerning the magnetic domains structure we have obtained that:

1. starting from the point $x=0$ up to the point $x_{zr} = 0.98$ there is a region in which $\sigma_{zz}(x)$ is the component with the highest value and it is positive (zone I).

2. and from this point to the point $x=1$ there is a second region, much narrower than the first one, in which $\sigma_r(x)$ is the highest positive stress component (zone II).

Using the relation [8]:

$$R_c / R_l = \left(M^* / M_s \right)^{1/2},$$

where $x_{zr} = R_c / R_l = 0.98$ from our numerical results we obtain the values of the reduce magnetization

$M^* / M_s = 0.96$. The high values of the reduced remanence makes these nanowires good candidates for sensing applications.

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