

SIMULATION OF MAGNETIZATION CURVES IN MAGNETIC THIN FILMS USING STONER-WOLFARTH MODEL

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Abstract. Computer simulation based on Stonner-Wolfarth model is used to simulate magnetization curves for Ni₈₀Fe₂₀ (Py) thin films and magnetic multilayers (MLs) with the structure Py/NM/Py where NM denotes a nonmagnetic layer. The results of computer simulations are compared with the magnetic measurements made with a Vibrating Sample Magnetometer (VSM).

Keywords: Thin films, Stonner-Wolfarth, Hysteresis loop

1. INTRODUCTION

In this study we used a micromagnetic simulator based on Stonner-Wolfarth [1] model to investigate the hysteresis loop of Ni₈₀Fe₂₀ (Py) thin films and Py/Cu/Py multilayers. The program, developed at NIST by Dr John Oti [2], calculate the interaction between the single-domains elements and the applied magnetic field. The element's magnetic properties, such as magnetization, anisotropy, pinning fields, must be specified or selected from a library of materials. The careful choice of the dimensions, the configurations and properties of elements permits the modelling of a wide range of technologically interesting systems.

2. THEORETICAL ASPECTS

In our approach the basic design unit is an *element* shaped as a rectangular prism. The element is oriented parallel to the coordinate axes of the system; the element may be *ferromagnetic* or *nonmagnetic*. The ferromagnetic element is a *single-domain element*, which means that it is uniformly magnetized and can thus be characterized by a single three-dimensional magnetization vector. The magnetization vector is free to rotate in three dimensions under the influence of magnetic fields. The equilibrium magnetization states of elements for static calculations are those that yield a minimum of the total free energy density of the system $E = \Gamma e_i$, where e_i is the free energy density of the element given by the expression [1-4]:

$$e_i = \frac{1}{2} \mathbf{M} \cdot \overline{\mathbf{N}} \mathbf{M} - \mathbf{H}_T \cdot \mathbf{M} \quad (1)$$

where the self-demagnetization tensor $\overline{\mathbf{N}}$ is expressed by a diagonal matrix whose nonzero elements (N_x, N_y, N_z ; $N_x + N_y + N_z = 1$) are the demagnetizing factors [2]. \mathbf{M} is the magnetization vector of the element and \mathbf{H}_T is the total effective field from all other sources excluding self-demagnetization. The first term on the right side of (1) represents the self-demagnetization energy of the element and the second term, the energy due to other magnetic interactions. The self-demagnetizing field sources for a uniformly magnetized element are the magnetic *surface charges* formed on its bounding faces. For a system composed of several elements, the field \mathbf{H}_T is a function of the magnetization of all elements of the system. This necessitates the use of self-consistent iterative methods in obtaining an energy minimum for the system [2]. This method finds the equilibrium magnetization orientation of an element. The updated magnetization values are used to recompute \mathbf{H}_T for each element, and this iteration procedure is repeated until the magnetization of the system reaches equilibrium. In the case of thin films we must consider a thin rectangular prism that lies in the xy plane. As we'll see, in this case, $N_z \approx 1$. This high value of the demagnetizing factor produces so called shape anisotropy. For example, if we consider a $10 \times 10 \mu\text{m}^2$ and 100 nm thick single-domain Permalloy thin film the self-demagnetization tensor becomes (N_x, N_y, N_z)=(0.017, 0.017, 0.966). The self-demagnetizing field under z direction (the shape anisotropy) is $H_D=760 \text{ kA/m}$, i.e. $H_D=9600 \text{ Oe}$. Because it is most suggestive in what follows we will use CGS units. On the other hand, the film may present an easy direction of magnetization defined by the direction of the anisotropy field, H_K . Usually, for Permalloy, $H_K=5 \text{ Oe}$. We present, in Fig. 1, the results of simulations made for a $10 \times 10 \mu\text{m}^2$ single-domain Permalloy thin film with a thickness of 100 nm and 10 nm respectively. From Fig. 1(a) we can see the importance of the demagnetizing fields in the film plane which produce a split of the M-H hysteresis loop under the hard axis. For a 10 nm thin film the demagnetizing coefficients are (N_x, N_y, N_z)=($1.84 \cdot 10^{-3}, 1.84 \cdot 10^{-3}, 0.998$) which lowers the demagnetizing fields in the film plane but enhances the demagnetizing field on a direction normal to the film plane. However, the thin film may have a complicated spin structure, not a single domain structure, in a way to reduce the dominant magnetostatic interactions. One example of the complicated spin structure is the magnetization curling formed at the edge of the layers [1].

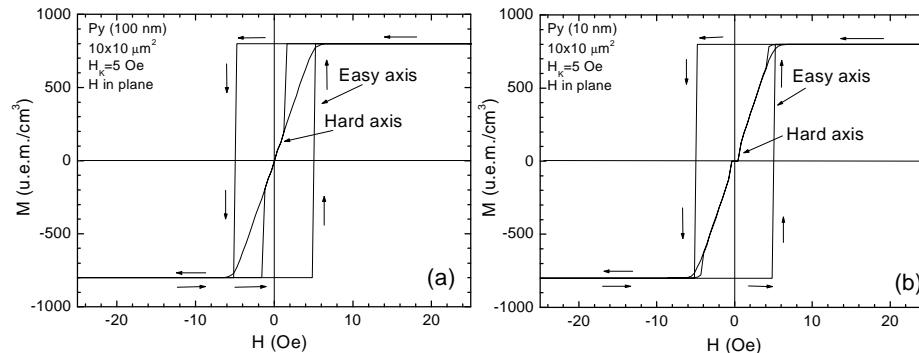


Fig. 1 - Simulation of M-H hysteresis loops for a 100 nm (a) and 10 nm (b) single-domain Permalloy thin film. The arrows are guides for the eyes.

For this reason we use a more realistic structure consisting in a number of single-domains which interact between them and with the applied magnetic field, like in Fig. 2.

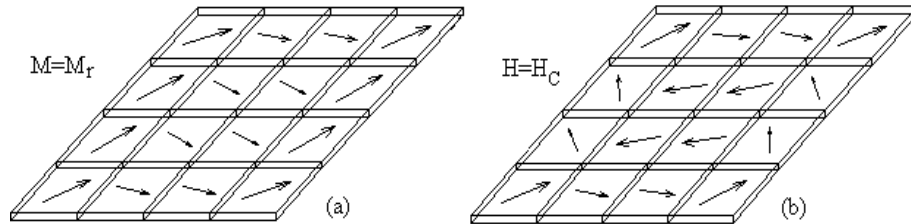


Fig. 2 - Spin structure resulting from our simulations for a 4x4 single-domains 10 nm thick Permalloy film in remanent state (a) and demagnetized state (b).

3. RESULTS AND DISCUSSION

In Fig. 3(a) we present the hysteresis loop measured with VSM for 100 nm thick Permalloy film deposited on to oxidized Si. The magnetic field is applied in the film plane. The AFM measurements reveal a surface with an average roughness of about 12.8 nm. The average grain size is 1 μm [5, 6]. Based on these data we used a structure of 4x4 single-domains 1 μm each side and 100 nm thick. The result of the simulation is presented in Fig. 3(b); the magnetic field is in the film plane. As we can see, for thick films (100 nm) the simulation gives only a qualitative result. The coercive field resulting from this simulation is $H_c \approx 50$ Oe which is much greater than the measured value that is about 3 Oe. For films with a thickness that exceed 100 nm the domain walls play a major role in the magnetization reversal process [1].

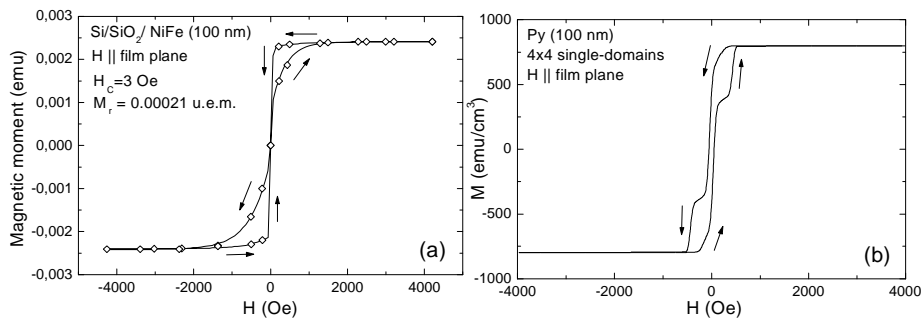


Fig. 3 - The hysteresis loop for a 100 nm thick Permalloy film measured with VSM (a) and the results of the micromagnetic simulation (b).

When the magnetic field is applied normal to the film plane the reversal process is a coherent rotation one as predicted by the Stoner-Wohlfarth model. In this case the

demagnetizing field plays the role of an anisotropy field, $H_K=9600$ Oe. The measured [6] and simulated magnetization curves with the field normal to the film plane are presented in Fig. 4.

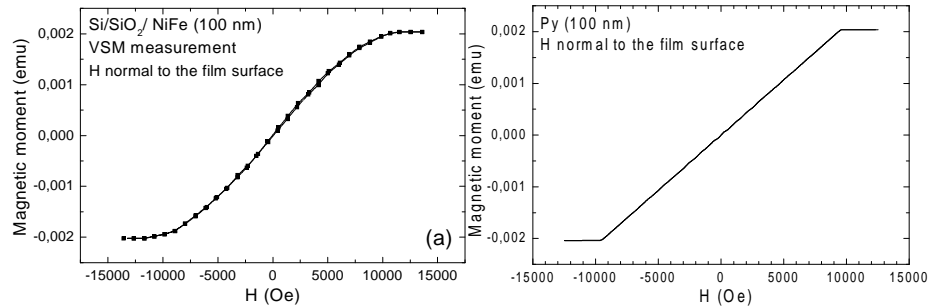


Fig. 4 - The hysteresis loop for a 100 nm thick Permalloy film measured with VSM (a) and the results of the micromagnetic simulation (b); the magnetic field is normal to the film plane.

The good agreement between the measured and the simulated loops reveals a relatively flat surface of the deposited film so the demagnetizing factor, N_z , has the value estimated by the theory $N_z=0.966$. For thin films the surface is very rough when the thickness is less than 5 nm. This will produce a reduction of the perpendicular anisotropy [5] and the demagnetizing factor N_z decreases. As a result the field for saturation in the out of plane configuration is less than the value predicted from the shape anisotropy (10 kOe).

When the magnetic films are thinner than 100 nm the energy due to the domain walls increases and the magnetization reversal mechanism is mainly due to rotation of the magnetic moments. We have simulated the magnetisation curve for a 10 nm thick Py film using a collection of 12x12 single domains. Each single domain is 10 nm thick and 95 nm each side. The distance between the adjacent domains is 5 nm. This model was inspired from the film structure [6]. The spin structure for the coercive field, H_C , and the magnetization curve are presented in Fig.5.

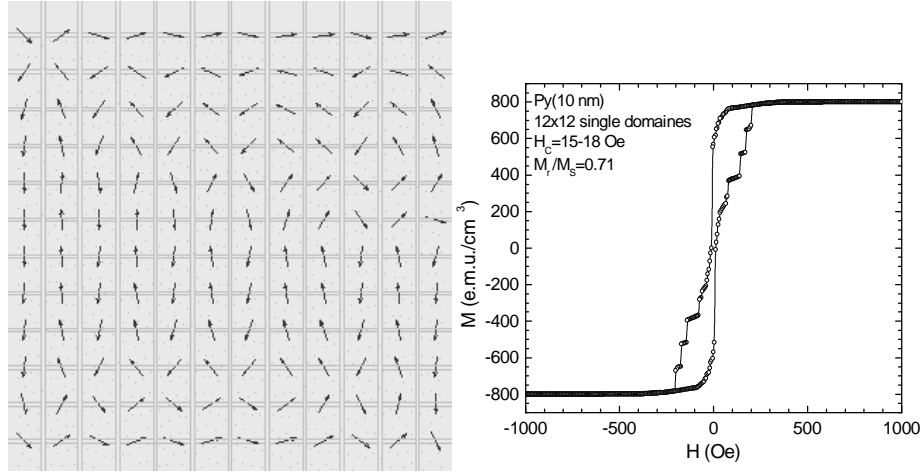


Fig. 5 - The results of the micromagnetic simulation for an evaporated Py(10 nm) thin film. The magnetic field is applied in the film plane.

The results are in good agreement with other experimental data [4-6], for the remanent-to-saturation magnetisation ratio $M_r/M_s \approx 0.71$, and with the MR measurements for the value of the coercive field, $H_C = 15$ Oe.

When we have to simulate the hysteresis loop for a multilayer structure (ML) we must consider the coupling between the ferromagnetic layers through the nonmagnetic layer. Let's consider the structure Py(10 nm)/Cu(4 nm)/Py(10 nm) which presents a hysteresis loop like in Fig. 6(a). To simulate the magnetisation curve we used two Py layers each consisting in a collection of 10x10 single domains of Py. Each single domain is 10 nm thick and 95 nm each side. The distance between the adjacent domains is 5 nm. The model was inspired from the film structure. The interlayer thickness is $t_{Cu} = 4$ nm. The coupling constant J , for $t_{Cu} > 1.5-2$ nm, is well described by the Néel model for positive magnetostatic interlayer coupling [7]:

$$J = \frac{\pi^2}{\sqrt{2}} \frac{h^2}{\lambda} \mu_0 M_S^2 \exp\left(\frac{-2\pi\sqrt{2}t_{Cu}}{\lambda}\right) \quad (2)$$

M_S is the saturation magnetization ($M_S = 800$ kA/m or 800 emu/cm³ in CGS). Here λ is determined by the grain size and h by the film roughness [7]. From AFM measurements [6] we have $h = 1.35$ nm and $\lambda = 15$ nm. The interlayer coupling is $J = 0.23$ mJ/m² and the resulting coupling field is $H_0 = 2457$ A/m (31 Oe). Because of Py bridges that exist through the spacer the coupling may have local variations that exceed 31 Oe [7]. Between the top and the bottom layers we introduced coupling fields that have random values from 30 to 60 Oe. The results of our calculations are presented in Fig. 6(b).

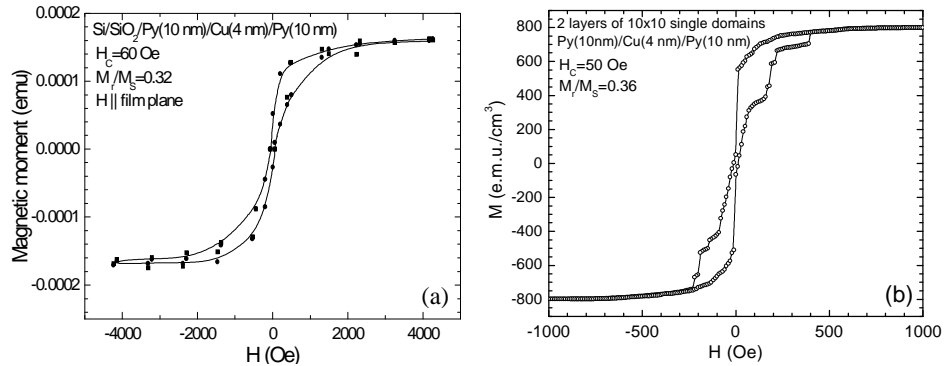


Fig. 6 - The hysteresis loop for a Si/SiO₂/Py(10 nm)/Cu(4 nm)/Py(10 nm) ML measured with VSM (a) and the results of the micromagnetic simulation (b); the magnetic field is in the film plane.

The agreement with the VSM measurement is very good. As we can see for our ML the ratio $M_r/M_s \approx 0.4$ is smaller than the value $M_r/M_s \approx 0.7$ obtained for a Py(10 nm) layer.

4. CONCLUSIONS

Computer simulation based on Stonner-Wolfarth model was used to investigate the magnetic hysteresis loops in thin films and magnetic multilayers. This method can be a very useful tool in the design process of a wide range of technologically interesting systems.

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