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COMPUTER SIMULATION OF MAGNETIZATION CURVES IN MAGNETIC THIN FILMS

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Computer simulation based on Stonner-Wolfarth model is used to investigate magnetization flop in magnetic thin films of $Ni_{80}Fe_{20}$ (Py) and magnetic multilayers with the structure Py/Cu/Py. The results of computer simulations are compared with the magnetic measurements made with a commercial Vibrating Sample Magnetometer (VSM).

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1. Introduction

Currently there is much interest in the transport and magnetic properties of metallic multilayer systems since the discovery of the giant magnetoresistance (GMR). Usually, the magnetic properties of the thin films are investigated using a Vibrating Sample Magnetometer (VSM) or other methods like Kerr magnetometry. In this study we use a micromagnetic simulator based on Stonner-Wolfarth [1] model to investigate the hysteresis loop of $Ni_{80}Fe_{20}$ (Py) thin films and Py/Cu/Py multilayers. The program, developed at NIST by Dr John Oti [2], calculates 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 permit 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 properties of the elements and the interactions between them are specified by the user. To obtain the response of the system, the used method is an energy minimization calculation in which an energy minimum is calculated for the system for a given value of applied 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 $E = \sum e_i$, where e_i is the free energy density of the element given by the expression [1-4]:

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$$e_i = \frac{1}{2}\boldsymbol{M}\cdot\overline{\boldsymbol{N}}\boldsymbol{M} - \boldsymbol{H_T}\cdot\boldsymbol{M} \tag{1}$$

where the self-demagnetization tensor $\overline{N}$ 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 of a uniformly magnetized ellipsoid with the same aspect ratio and principal axes (x, y, z) as the element. Such an ellipsoid is called an *equivalent ellipsoid* of the element. $\boldsymbol{M}$ is the magnetization vector of the element and $\boldsymbol{H_T}$ is the total effective field from all other sources excluding self-demagnetization. The first term on the right side of Eq.(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 $\boldsymbol{H_T}$ 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. During iteration, the magnetizations of the elements are rotated in a manner that minimizes their local free energy densities given by Eq.(1). This is accomplished by using a numerical implementation of the classical Stoner-Wohlfarth model that is applicable to general single-domain ellipsoids. This method finds the equilibrium magnetization orientation of an element. The updated magnetization values are used to recompute $\boldsymbol{H_T}$ 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. In this case, $N_z \approx 1$. The high value of the demagnetizing factor produces so called shape anisotropy. For example, if we consider a 10×10 μm^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 kA/m, i.e. H_D=9600 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 Oe. We present, in Fig. 1, the results of simulations made for a 10×10 μm^2 single-domain Permalloy thin film.

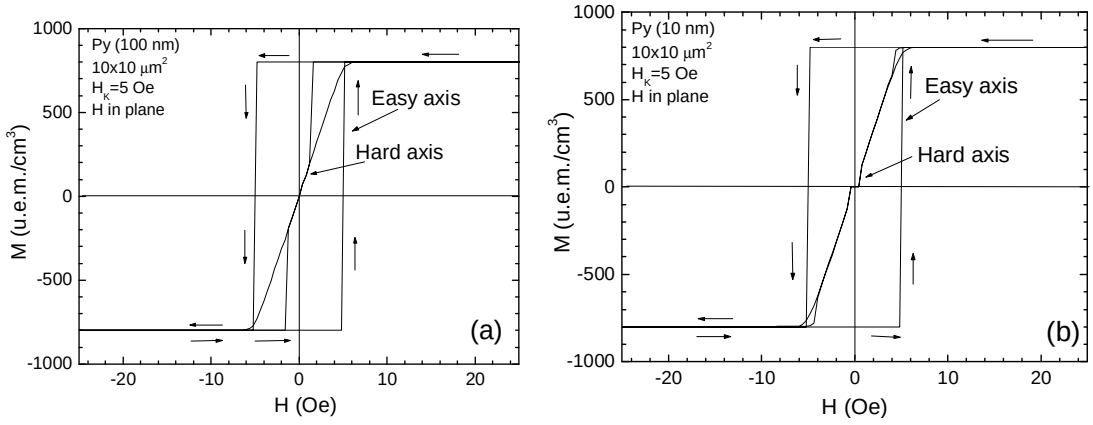

Fig. 1. Simulation of M-H hysteresis loops for a 100 nm (a) and 10 nm (b) single-domain Permalloy thin film. The arrows are guides for the eyes.

From Fig. 1(a) we can see, also, 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)=(1.84×10^{-3}, 1.84×10^{-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]. For this

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

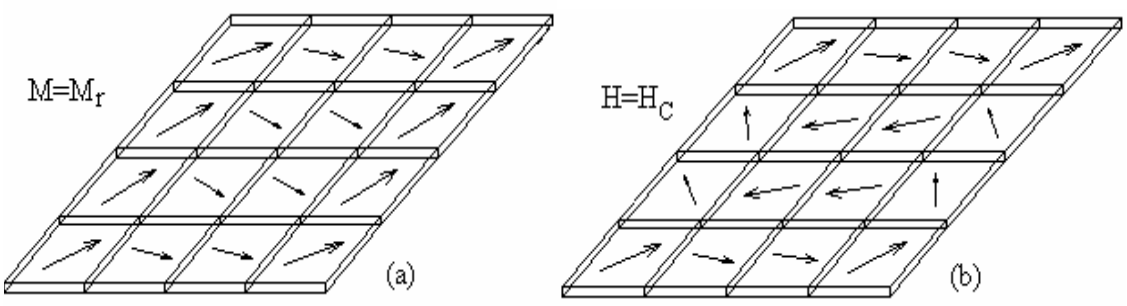

Fig. 2. Spin structure resulting from our simulations for a 4 × 4 single-domains 10 nm thick Permalloy film in remnant state (a) and demagnetized state (b).

3. Results and discussion

In Fig. 3(a) we present the hysteresis loop measured with VSM for a Permalloy thin film 100 nm thick, deposed 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 4 × 4 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.

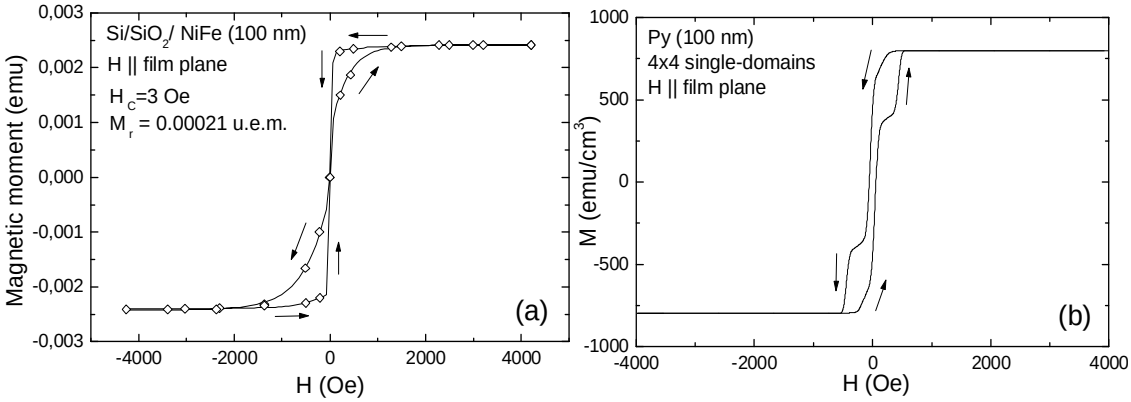

Fig. 3. The hysteresis loop for a 100 nm thick Permalloy film measured with VSM (a) and the results of the micromagnetic simulation (b).

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]. When the magnetic field is applied normal to the film plane the reversal process is 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.

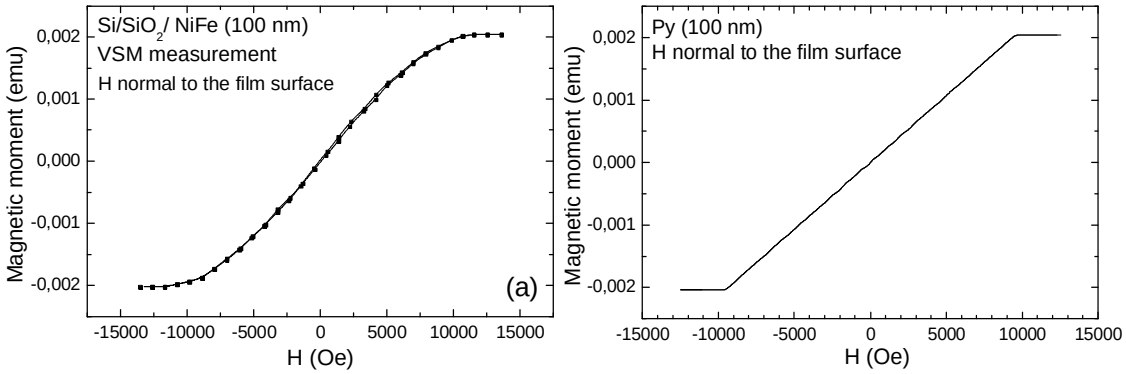

Fig. 4. The hysteresis loop for a 100 nm thick Permalloy film measured with VSM (a) and the results of the micromagnetic simulation (b); the magnetic field is normal to the film plane.

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 [5, 6] and in some cases the average roughness can exceed the film thickness. This will produce a reduction of the perpendicular anisotropy and the demagnetizing factor N_z decreases. As a result, the field for saturation in the out of plane configuration is less than predicted from the shape anisotropy (10 kOe). When the magnetic films are thinner than 100 nm the energy due to the domain walls increases. From this reason, for thin films, the magnetization reversal mechanism is mainly due to rotation of the magnetic moments. In Fig. 5 we present the simulation results with the magnetic field in plane for a structure of 4 × 4 single-domains 1 μm each side and 10 nm thick. Again, the domain size was inspired by the AFM measurements made on Si/SiO_2/Py(10 nm) system [6].

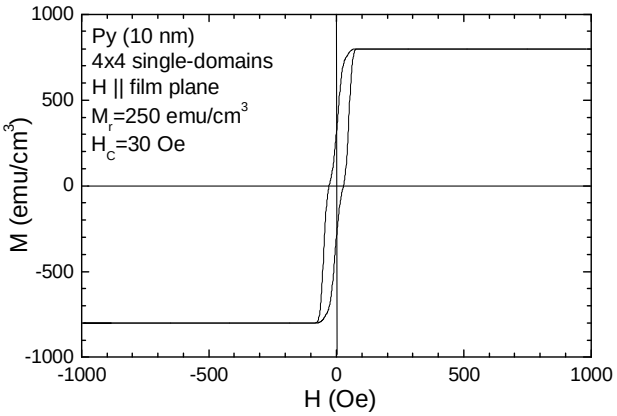

Fig. 5. The micromagnetic simulated hysteresis loop for 4x4 array 10 nm thick of Permalloy.

The value of the coercive field, H_C=30 Oe, is in good agreement with the experimental data reported elsewhere [1, 5] and with the magnetoresistive effect measurements. The spin structure and the magnetization curling formed at the edge of the layer were illustrated in Fig. 2. The formation of the closure structure in the demagnetized state is illustrated in Fig. 2(b).

The situation is a little more complicated when we have to simulate the hysteresis loop for a multilayer structure (ML) of the form Py/Cu/Py because we must consider the coupling between the ferromagnetic layers through the nonmagnetic layer (Cu). This coupling depends on the thickness of Cu, substrate (t_{Cu}) on its quality and on the deposition technique. We used thermal deposition to growth structures of the form $Si/SiO_2/Py(t_{Py})/Cu(t_{Cu})/Py(t_{Py})$ where t_{Py} was ranged between 4 and 10 nm and t_{Cu}=4, 8 nm. For t_{Py}=4 nm and t_{Cu}=4 nm the multilayer structure is not well defined because of the large roughness of Py layers, in the first stage of growing, and consequently the structure presents intermixing regions between Py and Cu at the interfaces. The M-H hysteresis loop is highly

distorted [6]. When the thickness of the Py layer increases to 10 nm, the roughness decreases and the ML structure is well defined. An interesting structure seems to be Si/SiO_2/Py(10 nm)/Cu(4 nm)/Py(10 nm) which presents a hysteresis loop like in Fig. 6(a). The result of the micromagnetic simulation is presented in Fig. 6(b). The coercive field obtained from the simulation is $H_C \approx 50$ Oe. The ratio between the remnant magnetization (M_r) and the saturation magnetization (M_S) is 0.22 from simulation and 0.29 from VSM measurements.

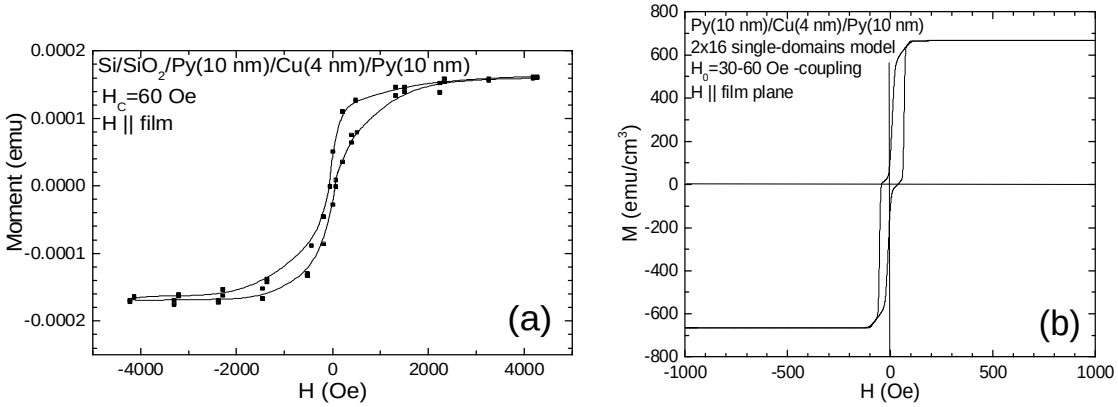

Fig. 6. The hysteresis loop for a Si/SiO_2/Py(10 nm)/Cu(4 nm)/Py(10 nm) ML measured with VSM (a) and the results of the micromagnetic simulation (b); the magnetic field is in the film plane.

These types of MLs exhibit a ferromagnetic interlayer coupling. It was shown [7] that the dependence of the coupling constant J on the Cu-layer thickness, for $t_{Cu}>1.5$-2 nm, is well described by the Néel model for magnetostatic interlayer coupling, based on the interaction between the dipole fields produced by rough interfaces:

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

Here, λ and h are the lateral length scale and amplitude of the roughness, respectively, and M_S is the saturation magnetization (M_S=800 kA/m or 800 emu/cm^3 in CGS). In this model the roughness is assumed to be two-dimensional and sinusoidal. Here, λ is determined by the grain size. From AFM measurements [6] we have h=1.35 nm and λ=15 nm. If we consider t_{Cu}=4 nm the interlayer coupling is J=0.23 mJ/m^2. For this value the coupling field is H_0=2457 A/m (31 Oe). This value is correct only if we consider the magnetic layers completely separated by the Cu spacer. Because of Py bridges that exists trough the spacer the coupling may have local variations that exceed 31 Oe. For this reason, in our simulation we consider two arrays of 4x4 single domains of Py(10 nm) separated by a 4 nm nonmagnetic layer. Between the top and the bottom layers we introduced coupling fields that have random values from 30 to 60 Oe.

Finally, if we suppose flat surfaces and spacer with a thickness $t_S>1.5$-2 nm between the layers it appears a negative magnetostatic coupling. For example this is the case of $Py/Al_2O_3/Py$ tunnel junction which is very attractive as a magnetic sensor. We present, in Fig. 7, the micromagnetic simulation for this ML and in Fig. 7(b), the spins configuration, for H≈35 Oe.

When |H|<150 Oe the negative magnetostatic coupling starts to rotate the spins in a manner so as to minimize the total free energy. For |H|<5 Oe the spins are antiparallel oriented so the total magnetization is 0.

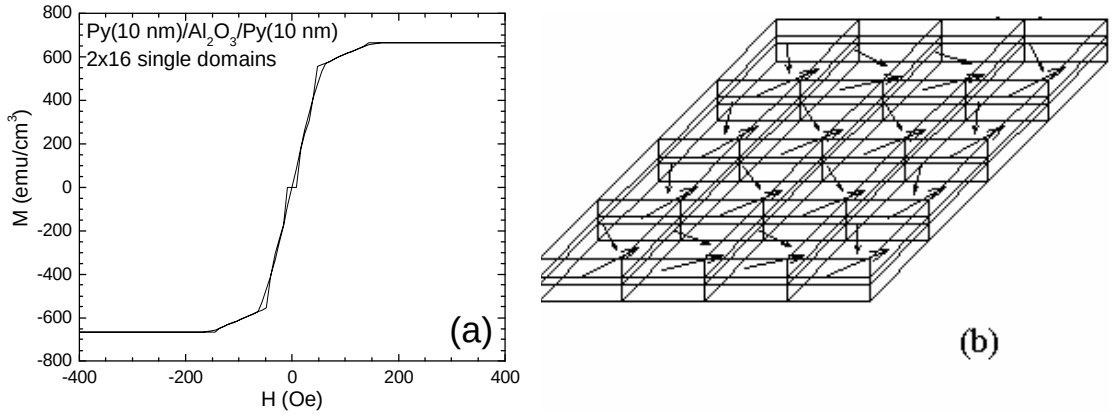

Fig. 7. The micromagnetic simulated loop (a) for a $Py/Al_2O_3/Py$ ML and the spins configuration (b) when H≈35 Oe. The magnetic field is in the film plane.

4. Conclusions

Computer simulation based on Stonner-Wolfarth model was used to investigate the magnetic hysteresis loops in thin films and magnetic multilayers. The results are in good agreement with the experimental data when the film thickness is below 100 nm. This method can be a very useful tool in the design process of a wide range of technologically interesting systems.

References

[1] R. F. Soohoo, Magnetic Thin Films, Harper and row, New York, 1965.
[2] John O. Oti, SimulMag Version 1.0, *Micromagnetic Simulation Software*, User's Manual, Electromagnetic Technology Division, National Institute of Standards and Technology Boulder, Colorado 80303, December 1997.
[3] M. Urbaniak, T. Lucinski, F. Stobiecki, J. Magn. Magn. Mater. **190**, 187 (1998).
[4] M. Labrune, J. C. S. Kools, A. Thiaville, J. Magn. Magn. Mater. **171**, 1 (1997).
[5] T. Lucinski, G. Reiss, N. Mattern, L. van Loyen, J. Magn. Magn. Mater. **189**, 39 (1998).
[6] J. Neamtu, M. Volmer, A. Coraci, Thin Solid Films **343-344**, 218 (1999).
[7] J. C. S. Kools, Th. G. S. M. Rijks, A. E. M. De Veirman, R. Coehoorn, IEEE Trans. Magn. **31**, 3918 (1995).