Micromagnetic simulations of magnetoelastic heterostructures

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Abstract: The system formed by a 10 nm thin film of Ni and a 10 μm-thick V_2O_3 layer shows a reversible enhancement of the coercivity ($\sim$300%) due to the structural phase transition (metal/insulator) of the V_2O_3layer. Performing micromagnetic simulations and comparing the results with experimental data we have studied the coupling mechanism on the Ni/V_2O_3 interface. We have proven that this coupling is responsible for the coercivity enhancement and that the magnetisation domains in the Ni do not follow exactly the metal/insulator domains on the V_2O_3. Finally, we have determined that the results of the simulations are in agreement with a phase coexistence in V_2O_3.

I. INTRODUCTION

Since the last part of the XX century, the world has experienced an unprecedented technological revolution. Throughout this process, the development of materials with emergent properties and novel functionalities has been responsible for many major scientific breakthroughs [1].

In the case of magnetic materials, a novel interesting approach is being able to control the magnetic properties of a material by other means rather than the application of a magnetic field; e.g. light, pressure or an electric field. The manipulation of magnetic properties without the application of a magnetic field opens the door for a completely new range of devices and possibilities [2].

In this regard, we address this issue by studying the properties of the heterostructure formed by a thin layer of Ni (10 nm) deposited onto another layer of 100 nm-thick vanadium oxide (V_2O_3). V_2O_3 undergoes a structural phase transition (SPT), from a rhombohedral structure at the high temperature phase, to a monoclinic phase at low temperature. Since the volume of the low temperature phase is 1% bigger than the high temperature phase, the SPT induces a strain in the Ni layer across the interface with the V_2O_3. This interficial strain produces a lattice deformation on the Ni layer which, due to its magnetoelastic characteristics, induces the formation of a magnetic anisotropy direction. This crystallographic structure change in V_2O_3 results in a remarkable and reversible modification of the Ni magnetic properties such as a large enhancement of coercivity in a narrow temperature range across the SPT [2][3].

However, a complete microscopic study of the magnetoelastic coupling in Ni/V_2O_3 is still lacking. Experimentally, this problem has been addressed at the group of Magnetic Nanomaterials, UB, by imaging the Ni magnetic domains as a function of temperature across the V_2O_3 SPT. This TFG represents a new approach to the problem, micromagnetic simulations.

The goal of this TFG is to use micromagnetic simulations to deepen our understanding on this topic.

II. SAMPLES AND EXPERIMENTAL CHARACTERISATION

Bilayers of 5nm Al/10nm Ni/100 nm V_2O_3 were prepared using magnetron sputtering deposition by our collegues at USCD, as described elsewhere [2]. [3](Fig.1).The Ni layer is polycrystalline, smooth (roughness of about 2 nm) and metallic. Macroscopic magnetic measurements show an increase of about 300% of the coercive field at the low-temperature phase (Fig.2).

A microscopic, magnetic characterization of the sample has been carried out by the advisor and coworkers by synchrotron-based photoemission electron microscopy (PEEM) combined with X-ray magnetic circular dichroism (XMCD) [4]. The temperature-driven variation of the FM domain structure of Ni (10 nm-thick) was mapped across the SPT of V_2O_3. It was observed that the initial ferromagnetic (FM) saturated state splits upon crossing the SPT into a pattern of small domains which reverse by progressive rotation. The fraction of such inverted domains monotonically grows across the SPT with the predominance of one of the coexisting structural phases, in agreement with the evolution of the insulator/metal transition in the V_2O_3 thin film [5]. It was observed that the Ni domains form stripe patterns with length and periodicity consistent with the nanotexture of the metal/insulating domain in the adjacent V_2O_3 film [4].

The main objective of this TFG is to gain further insight on the microscopic Ni/V_2O_3 coupling mechanism by performing micromagnetic simulations of our 10 nm-thick Ni layer under comparable experimental conditions and geometry used in the PEEM experiments. Simulation has proven itself a very useful tool in order to de-

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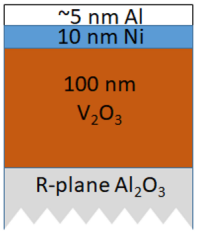

FIG. 1: Schematic representation of the samples used in the experimental measurements.

termine which parameters are important in the system and which of them are not. Furthermore, through simulation experiments we can measure the effect that has on the system a change in some of the parameters that are difficult to disentangle through the experimental measurements.

III. SIMULATIONS

The simulations were carried out using the object oriented micromagnetic computational framework (OOMMF), which is a project developed by the National Institute of Standards and Technology (NIST)[6]. However, some extra work has been done using python code in order to process the output data from the simulations and to provide the input data, depending on the simulation experiment carried out at each point of the research.

The phase transition in V_2O_3 is carried out inhomogeneously, following a very characteristic pattern (Fig.5c). Because of this pattern formation, the anisotropy induced in the Ni layer is neither homogeneous nor absolutely random. Thus, the different magnetisation domains that appear in the Ni, due to the induced anisotropy, follow a similar pattern, as will be discussed later.

The simulations performed during this work, and presented in this TFG, are mostly of two types. On one hand, several hysteresis loops of the Ni layer have been measured for each temperature aiming to understand the behaviour of the coercivity of the system with temperature. On the other hand, the magnetisation of the system has been homogeneously oriented in a certain direction and a constant magnetic field (200 Oe) has been applied anti-parallel to this direction (Fig.2a) to study the relative rotation of the system as a function of the temperature under this particular protocol matching that of PEEM experiments.

A uniform exchange constant of $3.4 \cdot 10^{-12}$ J/m has been used. In addition, an easy axis of magnetisation was introduced in the Ni layer in the x direction with an anisotropy constant of 2470 J/m^3 [3]. OOMMF computes the state of the system dividing it in cells of controllable dimensions distributed in a mesh. For each cell, the magnetisation is considered to be constant and the interactions with its neighbours are taken into account, as well as other long range parameters. The evolution of the system is controlled throughout iterations by the Landau-Lifshitz-Gilbert equation:

$$\frac{d\vec{M}}{dt} = -|\vec{\gamma}|\vec{M} \times H_{eff} + \frac{\alpha}{M_S}\left(\vec{M} \times \frac{d\vec{M}}{dt}\right) \quad (1)$$

where γ is the Gilbert gyromagnetic ratio, H_{eff} the effective field and α the damping constant, the Hamiltonian of the system is:

$$\mathcal{H} = \mathcal{H}_{Zeeman} + \mathcal{H}_{anisotropy} + \mathcal{H}_{exchange} + \mathcal{H}_{demag} \quad (2)$$

In this case a minimisation evolver has been chosen. This means that a stage in the simulation, such as e.g. a change in the applied magnetic field, is finished when the system reaches an equilibrium state. The equilibrium condition is reached when, after a recursive integration of eq.1, the energy does not significantly change, in other words, when the energy gets minimised for those particular conditions.[7]

A. Evolution of coercive field vs temperature

The so called coercivity is the strength of the magnetic field necessary to reduce to zero the magnetisation of the studied material and, thus, it is a useful measure of the *"magnetic hardness"* of a material. In order to determine the coercive field of the Ni, hysteresis loops as seen in (Fig.2b) were calculated for each temperature configuration.

For the simulations, a square mesh of $10\mu m$ x $10\mu m$ x 10 nm with 100 x 100 x 10 nm cells has been set, representing the thin-film nature of the Ni layer. In addition to the Ni magnetic anisotropy, the effect of the strain produced by the V_2O_3 needs also to be taken into account as schematically shown in (Fig1). With this in mind, an additional anisotropy of 20958 J/m^3 is introduced in the Ni layer forming an angle of 45° with the *"natural"* anisotropy axis of the Ni in the regions that are directly onto the domains of V_2O_3 that have transited to the low temperature phase. The values for both anisotropy constants were estimated from experimental data.

The OOMMF program reads the colour map from the experimental measurement of the V_2O_3, as will be shown later, and assigns the anisotropy values and directions according to the previously mentioned criteria. The regions presenting a white colour are assigned to the emergent red phase. The boundaries between the two phases in the V_2O_3 across the SPT (white colour) are assigned to the emergent red phase.

Due the limited experimental data available to feed the simulations (only five images corresponding to the con-

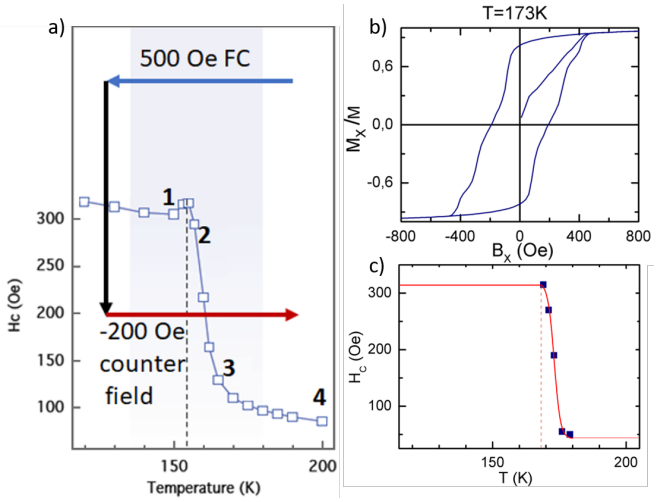

FIG. 2: **a)** Magnetic measurements of the coercivity of the system versus the temperature. **b)**A typical hysteresis loops used to calculate the coercivity of the system. **c)**Simulated coercivity vs temperature.

figuration of the V_2O_3) the data extracted from the simulation shows that the change in coercivity is observed (Fig.2c) and the change in the rotation angle of the magnetisation, when an external field is applied (Fig.4b), follows the same trend as in the experimental data (Fig.4a). This indicates that assuming that the strain produced by the phase coexistence in the V_2O_3 layer can explain the change in the magnetic properties of the Ni film.

Apart from the original image measured using PEEM, additional images were taken into account in order to gain additional statistical information. These extra images were made cutting the original image in 9 squares of the same size, rotating each piece randomly and composing an image of the original size from the pieces. All this process was carried out using a python script, and it was motivated by the impossibility of making new measurements of the real system. The result showed that the coercivity remains the same for all the created patterns studied. This indicate the lack of long range correlations in the formation of magnetic domains and that the only relevant feature, for the coercivity enhancement, is the width and the shape of the metal/insulator domains in the V_2O_3.

After all the process, the coercivity (H_C) data for 5 temperatures was successfully measured with an associated statistical uncertainty that proved itself too low to be noticed. The results are summarised in (Fig.2).

B. Rotation of the magnetisation under an external field

The above mentioned system, created with the simulation of the hysteresis loops in mind, presented itself as a valid tool for simulating other experiments with the Ni/V_2O_3 heterostructure. In this case, we will be studying the rotation of the magnetisation as a function of the temperature of the system under certain conditions. The following description corresponds to the simulation process; however, an analogous experiment was performed by the Nanomagnetic Materials group at Universitat de Barcelona. The data from these measurements are in good agreement with the data extracted from the simulation, which supports the idea that the simulations were using reasonable parameters.

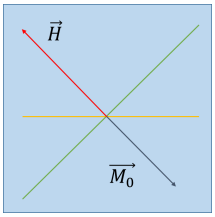

FIG. 3: Scheme illustrating the external field (red), the initial magnetisation (blue) and the anisotropy directions (yellow and green).

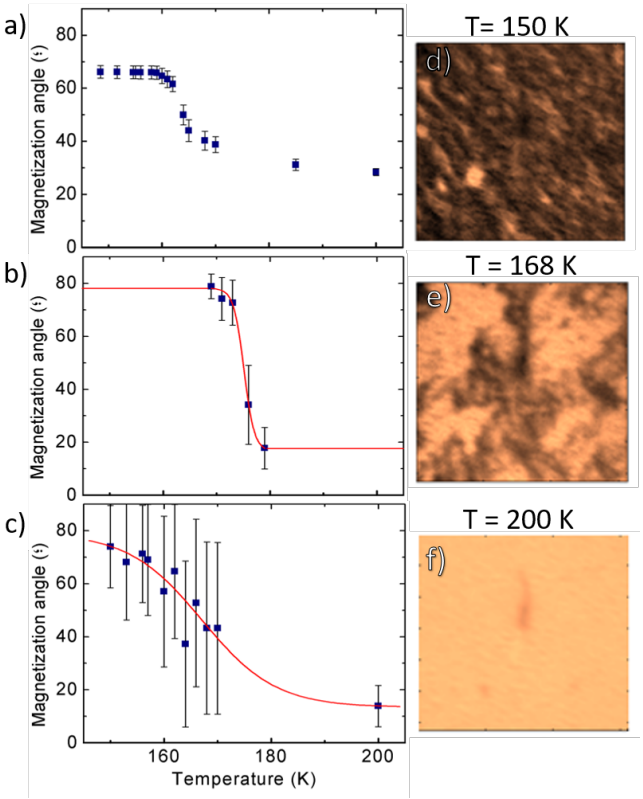

FIG. 4: **a)**Experimental average rotation of the Ni spins versus temperature across the SPT. **b)**Simulated average rotation of the spins. **c)**Simulated average rotation of the spins taking as input the distribution of the magnetisation domains measured in the Ni. **d),e),f)** Experimental measurements of the Ni magnetic domains using PEEM.

For this case, the initial magnetisation of the system

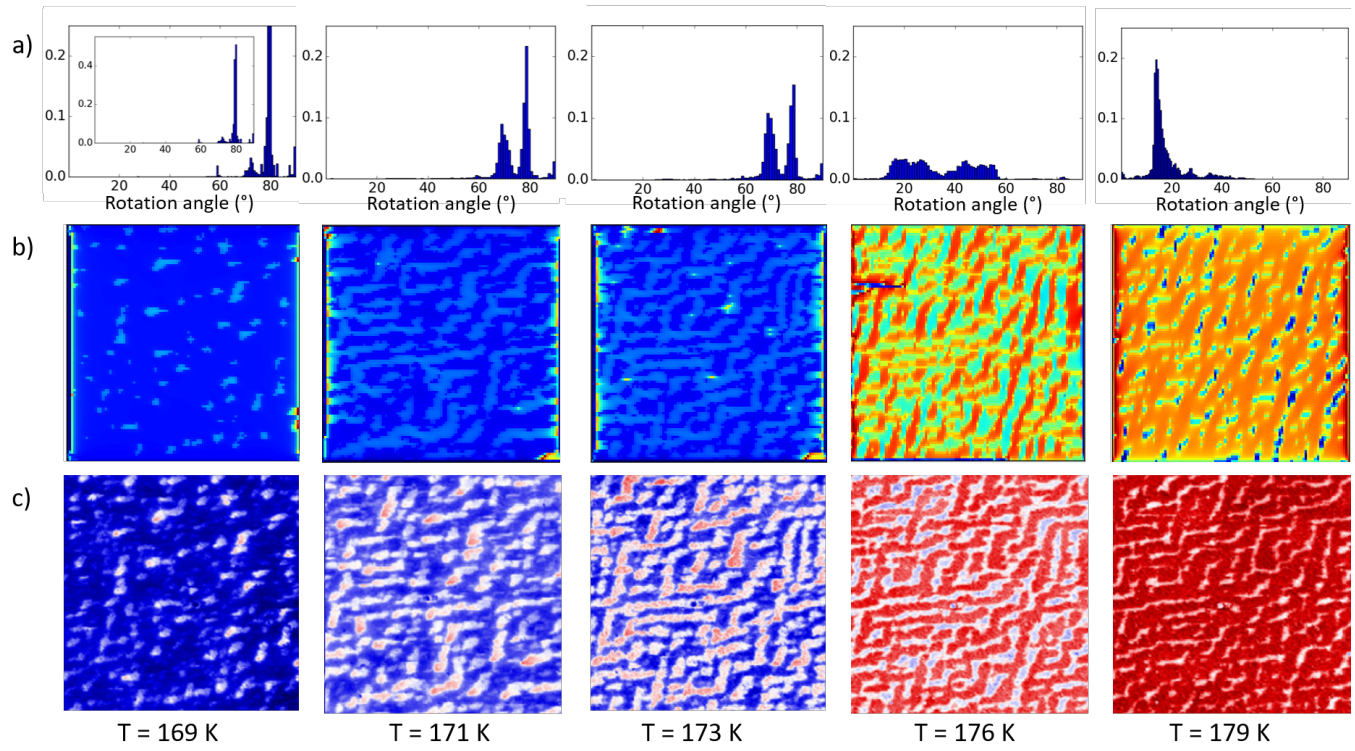

FIG. 5: **a)**Fraction of spins versus the rotation angle with respect the initial magnetisaton. **b)**Equilibrium configuration of the system. Blue and red regions indicate magnetisation in the direction of the applied field and the high temperature anisotropy. **c)**Image of the metal/insulator domains in V_2O_3 using scanning near-field optical microscope (SNOM). Blue and red regions stand for low (insulator) and high (metal) temperature phases across the SPT.

was set as the saturation magnetisation in a direction that forms an angle of 45° with the *"x"* axis (Fig.3). A constant magnetic field of 200 Oe was applied uniformly in the system in the opposite direction to the initial magnetisation (Fig.2a). Due to the effect of the magnetic field the magnetisation of the system rotated until the whole mesh reached the stationary state. The behaviour of the system was greatly influenced by the competing anisotropies introduced to simulate the proximity of the V_2O_3. In particular, the magnetisation exhibited different configurations for each temperature.

Apart from being able to accurately reproduce the conditions of previous measurements, additional aspects of the influence of the V_2O_3 layer in the behaviour of the Ni have been studied through simulation. In order to see with higher temperature resolution how the magnetic domains in the Ni are imprinted by the different structural V_2O_3 configurations across the SPT, the same kind of simulations were carried out using as input for the anisotropy distribution the experimental PEEM images of the Ni magnetic domains (Fig.4d-f) instead of the near-field optical microscopy of the metal/insulator domains in V_2O_3 (Fig.5c).

As can be seen in (Fig.4b-c), for high and low temperatures, the spins are oriented in the high temperature easy axis and the direction of the field respectively. This behaviour is due to the fact that the applied field is stronger

In the simulated system, the Ni thin film was divided into 100x100x10 nm cells and the magnetisation of the system was computed for each of the 10000 cells forming the mesh.The data of the average rotation angle of the spins with respect to their initial direction was calculated individually using a python script.

Evidence of phase coexistence has also been found, as presented for T=176K in (Fig.5a,b). The distribution of angles cover a wide range of values (from 10 to 60 degrees) and the image of the whole system contains regions of high and low temperature magnetisation.
than the low temperature anisotropy but weaker than the high temperature anisotropy. The narrow nature of the peaks and the global image of the spins confirm that for high and low temperatures the Ni layer presents a coherent magnetisation. Note that the tail in the right side of the angle distribution for T=179 is explained by considering the remaining low temperature domains.

IV. ORDER PARAMETER

The change in magnetisation of the Ni due to the V_2O_3 SPT can be regarded itself as a phase transition. Considering this, let us define an order parameter ϕ. The order parameter will take values from -1 to 1, being equal to 1 for the high temperature magnetisation (direction of

the high temperature anisotropy) and -1 for the low temperature magnetisation (in the direction of the applied field). Thus, the order parameter will be

$$\phi = \frac{1}{N}\sum^{N} a_i - b_i \tag{3}$$

where a_i and b_i are the absolute values of the projection of each spin in the high and low temperature directions and N is the total number of spins.

The behaviour of ϕ with respect to the temperature (Fig.6) is in good agreement with the data in (Fig.4b), which indicates that is an appropriate order parameter. Moreover, it is compatible with the phase coexistence because the standard deviation σ reaches its maximum in the middle of the SPF (Fig.6b). in good agreement with the wide distribution of metal/insulator domains in V_2O_3 shown in figure (Fig.5c).

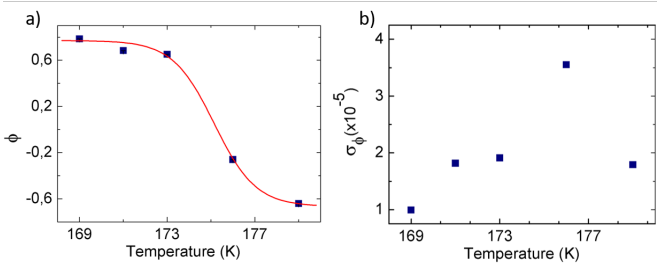

FIG. 6: **a)**Average order parameter versus temperature across the SPT. **b)**Standard deviation of the order parameter versus temperature.

V. CONCLUSIONS

- The simulations implemented with OOMMF have successfully reproduced the important microscopic features of the Ni/V_2O_3 heterostructure studied across the SPT. Our results indicate that the strain induced at the interface with V_2O_3 is responsible for the reversible enhancement of the coercive field of the Ni layer.

- The data of the rotation angle under the presence of a magnetic field provided by the simulations also reveals that magnetisation in the Ni film does not follow exactly the pattern induced by the V_2O_3. When the distribution of the anisotropy followed the configuration of magnetic domains in the Ni (Fig.4c) the results did not match the experimental data as well as they did when the anisotropy was introduced following the V_2O_3 phase configuration. Even though the high and low temperature phases were in agreement with the experimental data, the behaviour across the SPT was not reproduced.

- The spread in the distribution of the Ni magnetisation angles is very wide around the V_2O_3 SPT temperature and sharp far away from the transition (Fig.5a), in agreement with the phase coexistence in V_2O_3.

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[7] The criteria used to determine that the energy change is negligible can be specified by the user.