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Monte Carlo simulation of the magnetic exchange spring system DyFe$_2$(1) / YFe$_2$(4)

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Abstract. We investigate the magnetic properties of exchange coupled super-lattices constituted by a hard ferrimagnet DyFe$_2$ and a soft ferrimagnet YFe$_2$. The interface is characterized by a strong antiferromagnet due to the negative exchange couplings between the Dy and Fe magnetic moments. In this work, we reproduce hysteresis loops for the net and compound-specific magnetisations at different temperatures, by means of Monte Carlo simulations, and assess the quality of our results by a direct comparison to experimental hysteresis loops.

1. Introduction

Lave phase superlattices such as DyFe$_2$ / YFe$_2$ are interesting materials since they exhibit exchange spring properties [1]. They are exchange coupled systems constituted by a hard ferrimagnet (DyFe$_2$) whose magnetisation is dominated by the Dy moments, and a soft ferrimagnet alloy (YFe$_2$) in which Y carries a small moment antiparallel to that of iron [2]. The interface antiferromagnetic coupling (due to the negative exchange coupling between Dy and Fe moments) permits us to tailor extremely rich behaviours, such as exchange spring materials [1, 3]. In these hard/soft heterostructures, the classical magnetisation reversal process is expected to occur via the development of exchange springs in the soft part before the irreversible switch of the hard one. The magnetisation of the hard material remains tightly stuck by anisotropy, whereas the magnetic moments of the soft layer, locally pinned by exchange at the interfaces, may be rotated freely by the external magnetic field far from the pinning center. This simple description of magnetic exchange springs sometimes permits us to infer the magnetic profile from macroscopic magnetisation measurements [4]. The technological relevance of these materials ranges from applications as permanent magnets [5], as giant magnetoresistance (GMR) spin devices [6], to usage for advanced recording media [7]. In this paper, we report on the wide thermal evolution of the magnetisation reversal process in a super-lattice DyFe$_2$(5nm)/YFe$_2$(20nm), and we compare the experimental results to the simulation’s one by using the Monte Carlo method. These results have especially
revealed an unexpected high temperature situation, where magnetisation reversal first occurs in the harder DyFe$_2$ layers, and the magnetic springs are partly translated from inside the soft YFe$_2$ layers to the hard DyFe$_2$ ones.

2. Model and numerical simulations

Due to the many degrees of freedom of the spin system, we have chosen to use numerical methods in order to give a detailed microscopic description of the system. Since we are especially interested in the magnetisation reversal process we use Monte Carlo simulations in the canonical ensemble with time step quantification [8]. The model chosen is the classical Heisenberg model [9],

\[
H = - \sum_{<i,j>} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j - D(\text{Dy}) \sum_{i \in \text{Dy}} (\mathbf{S}_i \cdot \mathbf{x})^2 - D(\text{Y}) \sum_{i \in \text{Y}} (\mathbf{S}_i \cdot \mathbf{x})^2 - B \cdot \sum_{i} \mathbf{m}_i,
\]

where $\mathbf{S}_i$ are spin vectors at site $i$. The first term represents the exchange energy over nearest neighbours, the second and third sums represent an uniaxial anisotropy which favors the $x$ axis as the easy axis of the magnetisation and the last sum corresponds to the Zeeman interaction with the applied magnetic field. The values of the magnetic parameters have been estimated from experimental data concerning the Curie temperatures of the different species.

3. Simulated versus experimental results at low temperature

DyFe$_2$ / YFe$_2$ superlattices are characterized by a high Curie temperature ($T \sim 600$K) [10] due to the strong Fe-Fe exchange interactions. Moreover, the Dy-Fe exchange interactions give rise to antiferromagnetic couplings between the Dy and Fe moments which lead to ferrimagnetic structures when there is no magnetic applied field. At $T = 10$K, the experimental and numerical hysteresis loops are compared in Figure 1 for several superlattices of different thicknesses which exhibit three different behaviours [11, 12].

- The first behaviour is a DyFe$_2$ magnetically dominated behaviour obtained when the thickness of the hard layer (DyFe$_2$) is larger than the soft layer’s one ((1) and (4)). In this case, the loop is square as for a single hard phase, there is no signature of magnetic walls in the YFe$_2$ layers and the magnetisation reversal is completely governed by the anisotropy in the DyFe$_2$ layers. The giant ferromagnetic superlattice behaves as unique block with a one step magnetisation reversal, where the hard and soft magnetic layers switch as a unit.

- The second case corresponds to an almost magnetically compensated behaviour when the thicknesses of the layers are comparable ((2) and (5)). The measured hysteresis loops display a characteristic feature of magnetic exchange spring with
Figure 1. Experimental ((1), (2), (3)) [11, 12] and simulated ((4), (5), (6)) hysteresis loops of DyFe₂ / YFe₂ superlattices measured at low temperature (T = 10K). The magnetic behaviour of the samples is strongly related to the thickness of the layers: (1) - DyFe₂ (10nm)/YFe₂ (5nm); (2) - DyFe₂ (10nm)/YFe₂ (13nm); (3) - DyFe₂ (5.5nm)/YFe₂ (22nm). The figures with the experimental data ((1), (2), (3)) are shown with the permission of the authors.

The rise of an interface wall in the soft YFe₂ layer. The reversal of the magnetisation then occurs in two steps: firstly the rise of the interface wall, secondly the abrupt reversal of the hard DyFe₂ layer.

- The third behaviour is an YFe₂ magnetically dominated behaviour when the soft layer thickness is much larger than the hard layer one ((3) and (6)). In this case, various schematic spin configurations can be considered, as a function of the applied field. The thickness of the soft magnetic layer YFe₂ is so large relative to the hard layer that the reversal of the magnetisation occurs with a characteristic negative coercivity since the net magnetisation becomes negative even though the applied magnetic field is still positive.
4. Influence of the temperature for the DyFe$_2$(1)/YFe$_2$(4) superlattice

The experimental hysteresis loop of the sample DyFe$_2$(5nm)/YFe$_2$(20nm) at $T = 200K$ is shown in Figure 2 ((1)) from XMCD and macroscopic magnetisation measurements [4, 13]. As a comparison, we have also simulated the hysteresis loop of the DyFe$_2$(1)/YFe$_2$(4) superlattice ((6) in Figure 1) at $T = 200K$ ((2) in Figure 2). We observe that in both cases (experimental or simulated) the magnetisation reversal then occurs in a three step process and that the coercive field is positive contrary to the case at low temperature (Figure 1) or even at $T = 100K$.

Figure 2. Experimental hysteresis loop (1) of a DyFe$_2$(5nm)/YFe$_2$(20nm) superlattice obtained from XMCD and macroscopic magnetisation measurements [4, 13] and numerical hysteresis loop (2) measured at $T = 200K$. The figure with the experimental data ((1)) is shown with the permission of the authors.

Then, these results suggest a strong temperature dependence of the magnetisation reversal. In this sample, the YFe$_2$ magnetisation is dominant at all temperature but its influence becomes stronger when the temperature increases since the Dy magnetic moments become disordered. Thus, the reversal of the magnetisation evolves from a soft first mechanism below 200K (Figure 1) to a very unusual mechanism above this temperature, where the magnetisation reversal first affects the hard DyFe$_2$ layers, while the soft YFe$_2$ magnetisation remains aligned with the applied field direction. A sharp
transition between these two processes has been observed, that account for the thermal evolution of coercivity from a negative to a positive value.

5. Conclusion

In this article, it was shown that the Monte Carlo method, adapted to include magnetic exchange springs, can be used to provide a good semi-quantitative interpretation of DyFe$_2$/YFe$_2$ multilayers. In particular, we have been able to reproduce hysteresis loops with characteristics matching those of experimental work at different temperatures. The strong thermal dependence of anisotropy plays a key role for the reversal processes, and the interplay with exchange and Zeeman energy is understood on a qualitative level.

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