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A Monte Carlo study of the magnetization reversal in DyFe₂/YFe₂ exchange-coupled superlattices

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A B S T R A C T

Monte Carlo simulations are used to perform an atomic scale modeling of the magnetic properties of epitaxial exchange-coupled DyFe₂/YFe₂ superlattices. These samples, extremely well-researched experimentally, are constituted by a hard ferrimagnet DyFe₂ and a soft ferrimagnet YFe₂ antiferromagnetically coupled. Depending on the layers' thickness and on the temperature, the field dependence of the magnetization depth profile is complex going from a unique giant ferromagnetic block to exchange spring behavior when the soft YFe₂ layers reverse for positive bias fields. In some particular conditions of temperature and layers' thicknesses, it can even be easier to reverse the hard thin DyFe₂ layers for positive fields, while the soft thick YFe₂ layers keep their magnetization along the field. In this work, we reproduce by Monte Carlo simulations hysteresis loops for the net and compound-specific magnetizations at different temperatures, and assess the quality of the results by a direct comparison to experimental hysteresis loops.

1. Introduction

The study of exchange-coupled systems which combine two different magnetic materials that magnetically interact with each other at their interfaces has focused on an intense research activity for several years since they may exhibit interesting properties as spring magnet behavior and exchange bias effect [1]. Their potential application may concern permanent magnets [2] or data storage media [3,4] for example. These applications need a good understanding of the magnetization switching in exchange-spring structures for which the multilayered films of Laves phase REFe₂ (RE=rare earth) grown by molecular beam epitaxy are very good system models [5]. DyFe₂/YFe₂ superlattices are heterostructures that consist of hard DyFe₂ and soft YFe₂ ferrimagnetic layers. The hard magnetic phase tends to resist to magnetization reversal in high fields owing to its high anisotropy while the soft phase possesses large magnetization. There are three magnetic interactions that couple the moments of the rare earth and transition metal sites [6,7]. For DyFe₂, these are Fe-Fe interactions $J_{\text{Fe-Fe}}$, Dy-Fe interactions $J_{\text{Dy-Fe}}$ and Dy-Dy interactions $J_{\text{Dy-Dy}}$ with

$$J_{\text{Fe-Fe}} \gg -J_{\text{Dy-Fe}} > J_{\text{Dy-Dy}}$$

In the case of YFe₂ which is also ferrimagnetic but with a smaller induced moment essentially due to iron, its global magnetization is antiparallel to the one of DyFe₂ as qualitatively shown in Fig. 1(a). The simplest scenario used to describe the magnetization reversal in such a hard/soft coupled system is usually the formation of exchange springs in the soft material (Fig. 1(b)), before the irreversible switch of the hard material [1].

However, some experimental studies have shown that this very simple description of the magnetization reversal is not valid in some circumstances of relatively high temperature or thin magnetic hard DyFe₂ layers [6,8,9]. In that case, the magnetization reversal first affects the hard DyFe₂ layers whereas the YFe₂ magnetization remains *frozen* in the applied field direction. This scenario requires a decrease of the hard layers' anisotropy energy due either to the high temperature or to the thinness of the DyFe₂ layer.

These different experimental scenarios observed are the reason for which the numerical simulations at the atomic level may give a helpful tool to understand this wide variety of magnetic behaviors and are complementary to previous studies involving micromagnetic simulations [10].

2. Model and numerical simulations

We consider a face centered cubic (fcc) multilayered system made up of Fe, Dy and Y atoms. The direction of the uniaxial

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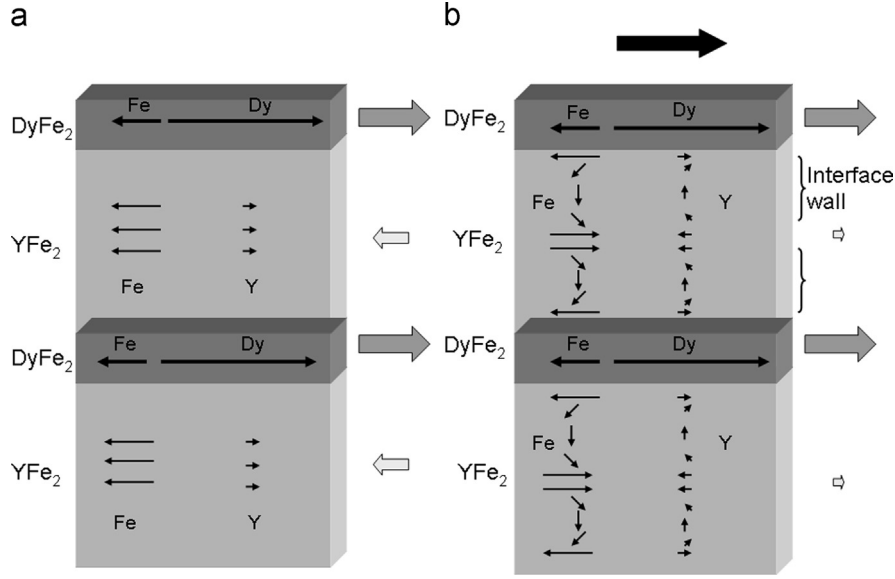


Fig. 1. Schematic view of the magnetization order in DyFe₂/YFe₂ superlattices ((a) fundamental state without magnetic field, $B=0$, (b) stable state with an applied magnetic field $B \neq 0$). The interface wall in the soft YFe₂ layers is visible when the magnetization turns plane by plane. Two bilayers are shown in each case.

anisotropy has been identified, in experimental superlattices, as the $[1 \bar{1} 0]$ in-plane direction whatever the temperature [11]. The SQUID measurements which the present work refers to have then been performed with an applied magnetic field along the same $[1 \bar{1} 0]$ direction.

The Monte Carlo method in the canonical ensemble is used to investigate magnetization reversal in order to give a detailed microscopic description of the system. This method is well-known to ensure a good convergence toward the thermodynamic equilibrium but it may in some circumstances not describe properly the magnetization reversal. So, we use here the algorithm proposed by Nowak et al. [12] with time step quantification. This technique allows us to get reliable Monte Carlo simulations with a reasonable number of Monte Carlo steps at low temperature. Moreover, unlike the standard Metropolis algorithm, this method prevents nonphysical spin flips by tunneling across the barrier. One Monte Carlo step (MCS) consists in examining all spins of the system once. At each temperature, 5000 MCSs were performed to reach the thermodynamic equilibrium, and afterwards the physical quantities were measured by averaging over the next 10 000 MCSs. The model chosen is the classical Heisenberg model

$$H = - \sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j - D(\text{Dy}) \sum_{i \in \text{Dy}} (\mathbf{S}_i \cdot \mathbf{x})^2 - \mathbf{B} \cdot \sum_i \mathbf{m}_i,$$

where \mathbf{S}_i are the spin vectors at site i . The first term is the exchange energy over nearest neighbors of the same or different species, the second sum represents a uniaxial anisotropy which favors the so-called x -axis (corresponding in fact to the $[1 \bar{1} 0]$ direction) as the easy axis of the magnetization and concerns only the Dy atoms. Indeed, the strong magnetic anisotropy in the hard layer is due to the interaction of the crystal field with the RE ions [13]. Finally, the last sum corresponds to the Zeeman interaction with the magnetic field applied in the easy $[1 \bar{1} 0]$ direction.

The values of the magnetic parameters have been estimated from experimental data relative to the Curie temperatures of the multilayers and from the configuration of the magnetic moments of the different species in the fundamental state (Fig. 1(a)). The magnetization of the individual layers has been estimated in these superlattices at $0.9 \mu_B/\text{at.}$ for the YFe₂ layers and $1.65 \mu_B/\text{at.}$ for the DyFe₂ layers [5]. These values are in good agreement with those used by Bowden et al. for their magnetic modeling [14]. We observe that, due to the antiparallel orientation of the

magnetization of the DyFe₂ and YFe₂ layers at low temperature, the ratio of the thicknesses which leads to a compensated magnetic state at $T=0$ and without any magnetic field is $e_{\text{DyFe}_2}/e_{\text{YFe}_2} = 0.5$. Finally, the estimated values of the first-neighbors exchange interactions, already used in previous studies of Fe–Dy multilayers [15] except those concerning the Y atoms, are given in Table 1.

3. Simulated versus experimental results

As described in Section 1, different magnetization reversal processes can occur in the exchange-coupled superlattices depending on the layers' thicknesses and on the temperature. We present here a detailed description of these behaviors, as they are obtained experimentally and can be reproduced and interpreted by Monte Carlo simulations.

3.1. Single-step reversal

A Rigid magnetic Block (RB) behavior when the switching is dominated by the hard DyFe₂ layer can be easily observed. The hysteresis loop is square and as for a single hard phase, there is no signature of magnetic walls in the YFe₂ layers; the magnetization reversal is completely governed by the anisotropy in the DyFe₂ layers. The giant ferromagnetic superlattice behaves as unique block with a one step magnetization reversal, where the hard and soft magnetic layers switch as a unit for a coercive field which strongly decreases when the temperature increases (Fig. 2).

It has to be noticed that if the qualitative thermal evolution of the magnetization reversal is correctly reproduced by the numerical simulations, the quantitative value of the simulated coercive field is clearly overestimated. This effect is attributed to the magnetic parameters, especially the anisotropy constant, whose temperature dependence is not included in the Monte Carlo procedure. Then, our model underestimates probably the decrease of the energy barrier between the two magnetized opposite states. This scenario can also be observed when the soft layer YFe₂ is thicker than the hard layer DyFe₂ but in the particular case of thin individual layer samples DyFe₂ (1 nm)/YFe₂ (4 nm) [6] such that the external magnetic field does not allow to break the ferrimagnetic configuration resulting from exchange. Indeed, in this case,

the YFe_2 layers are too thin to enable the development of magnetic walls. The large value of the coercive field has also to be noticed since at low temperature the ferrimagnetic configuration is maintained for a large negative field applied.

3.2. Two-step reversal

A two-step reversal can be observed with a Soft layers First (SF) switching and negative or positive coercivity. This scenario holds with an almost magnetically compensated behavior which is observed when the thickness of the soft layer is slightly larger than the hard layers one. In this superlattice, the DyFe_2 and YFe_2 net magnetizations can be almost equal and the ferrimagnetic arrangement stabilized after the first reversal step results then in approximately zero net moment (Fig. 3(1) and (2)).

From a general point of view, the measured hysteresis loops display a characteristic feature of magnetic exchange spring with the rise of an interface wall in the soft YFe_2 layer where their cost is expected to be the smallest, as qualitatively shown in Fig. 1(b). We observe a very good qualitative agreement between the experimental and simulated curves describing the reversal of the magnetization but a relative discrepancy from a numerical point of view concerning the coercive field and the zero-field behavior. The reversal of the magnetization then occurs in two steps: firstly the rise of the interface wall, secondly the abrupt reversal of the hard DyFe_2 layer. This scenario can even lead to the measurement

Table 1
Exchange interactions between nearest-neighbor atoms used in the simulations. The uniaxial anisotropy constant $D(\text{Dy})$ due to the RE contribution is also given.

Exchange interactions	$J_{\text{Fe-Fe}}/k_B$	$J_{\text{Fe-Dy}}/k_B$	$J_{\text{Dy-Dy}}/k_B$
	280 K	-41.75 K	6.5 K
	$J_{\text{Fe-Y}}/k_B$	$J_{\text{Y-Y}}/k_B$	$J_{\text{Dy-Y}}/k_B$
	-41.75 K	50 K	10 K
Anisotropy constant	$D(\text{Dy})/k_B = 2$ K		

of a negative coercivity and a negative remanence when the magnetization of the whole superlattice is governed by the soft layer contribution, i.e. for a significative thicker YFe_2 layer compared to the DyFe_2 layer (Fig. 3(3) and (4) where the soft YFe_2 layer is 4 times thicker than the hard DyFe_2 layer). But it has to be mentioned that this behavior is strongly dependent on the temperature since the DyFe_2 magnetization decreases more rapidly in temperature than the YFe_2 ones. Thus, the same samples at higher temperature (300 K for example) lead to a switching governed by the YFe_2 soft layer which becomes magnetically dominant. This influence of the temperature on the reversal mechanism is investigated in the next section.

3.3. Three-step reversal

A Hard layer First (HF) reversal when the soft layer thickness is much larger than the hard layers one can also be observed although it corresponds to a less usual situation (Fig. 4). Several schematic spin configurations can be considered in function of the applied field (Fig. 4(2)).

The description of the magnetization reversal process is evidenced by the measurement of the magnetization of the hard DyFe_2 and soft YFe_2 layers in the simulations (Fig. 4(3)).

This last situation is called Hard layer First (HF) switching since due to its small thickness, the anisotropy energy of the hard layer DyFe_2 is not strong enough to stabilize it at the beginning of the reversal. Then we observe a first switching of the DyFe_2 layers for a large magnetic field applied followed by the reversal of the magnetization of the whole sample at a low field and finally the second switching of the YFe_2 layers. Once again, the shape of the hysteresis loops is strongly dependent on the measurement temperature: when the temperature increases, the DyFe_2 reversal is easier and the whole multilayer reverses for a smaller negative field.

In order to get a more accurate knowledge of the localization of the interface wall, in the two last cases (SF and HF), we have

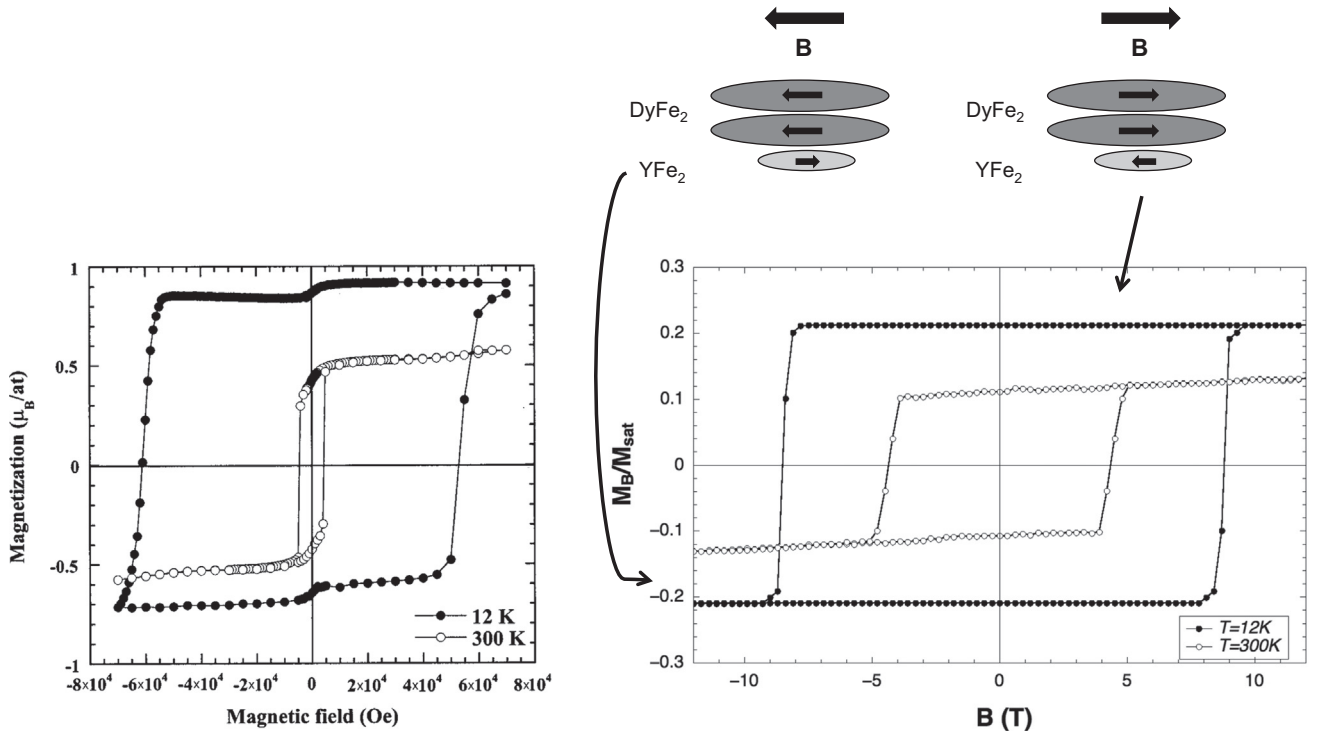


Fig. 2. Experimental (1) and simulated (2) hysteresis loops of DyFe_2 (10 nm)/ YFe_2 (5 nm) superlattices showing a Rigid magnetic Block behavior at low ($T=12$ K) and intermediate ($T=300$ K) temperatures [5].

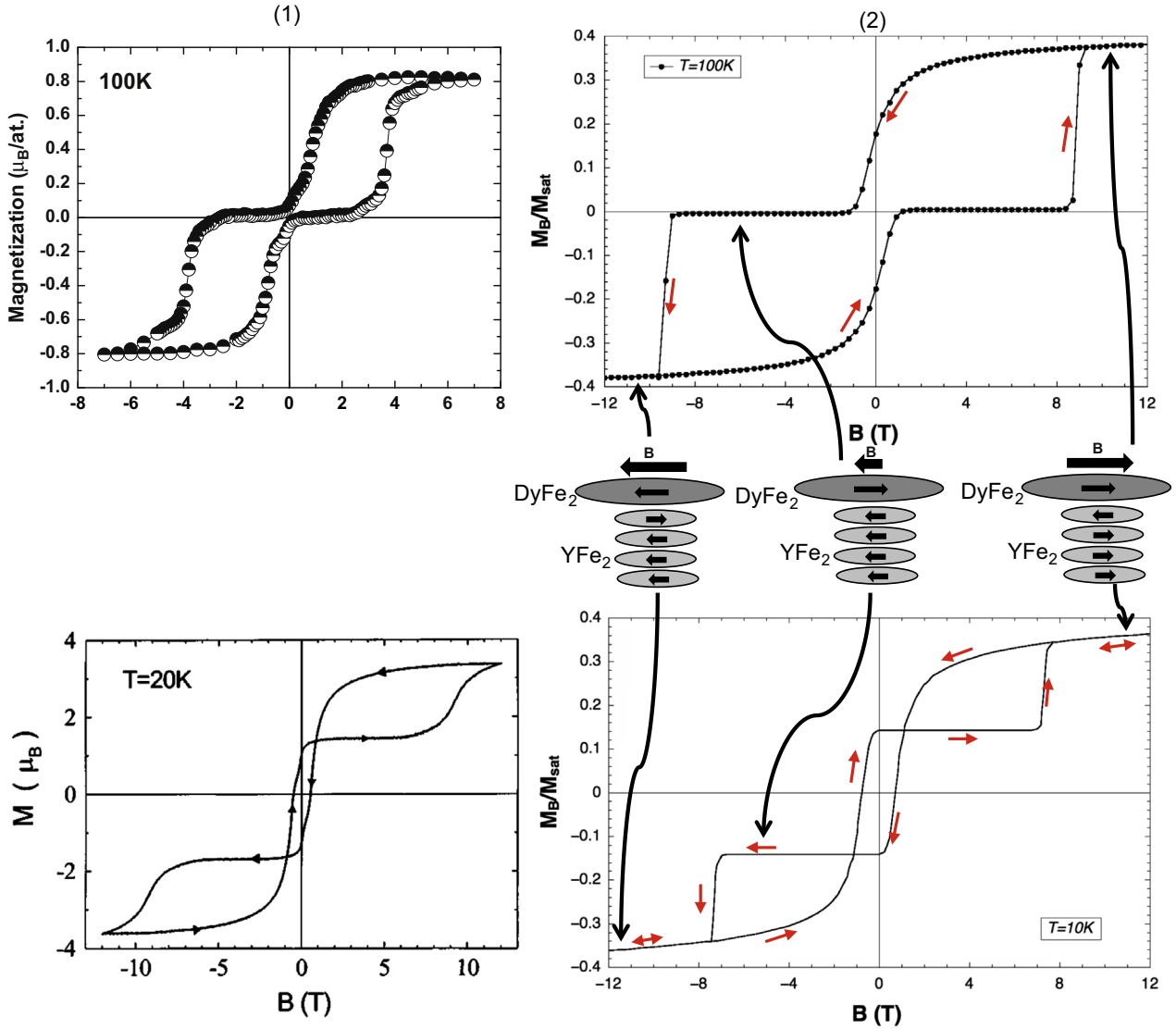


Fig. 3. Experimental (1) and simulated (2) hysteresis loops of DyFe₂ (10 nm)/YFe₂ (20 nm) superlattices describing a Soft layer First switching at $T=100$ K [6]; experimental (3) and simulated (4) hysteresis loops of DyFe₂ (5.5 nm)/YFe₂ (22 nm) superlattices characterized by a negative coercivity and a negative remanence at low temperature ($T=20$ K [16] or 10 K).

estimated, from the simulation data, the angle θ_B between the directions of the magnetization of each atomic plane and the applied magnetic field (Fig. 5).

In the ferrimagnetic state, when the DyFe₂ magnetization points up in the direction of the magnetic field whereas the YFe₂ magnetization is opposite, the angle θ_B is equal to 0 in the DyFe₂ layer and 180° in the YFe₂ layer. The result of the simulated multilayer is shown in Fig. 5 for a superlattice DyFe₂ (10 nm)/YFe₂ (20 nm) at low temperature ($T=10$ K).

We observe that the ferrimagnetic state is approximately reached only in the interface region and for a moderate applied magnetic field. Moreover, the interface wall, characterized by an angle different from 0 or 180° is essentially located in the soft YFe₂ layer with the magnetization of the core of the YFe₂ layer which points up in the direction of the magnetic field. However, the magnetization of the DyFe₂ atomic planes located near the interface is also disoriented relative to the field axis in order to satisfy the interface exchange couplings. These results are qualitatively in good agreement with previous experimental studies which show that for samples with rather thick individual thicknesses, the reversal of the magnetization is due to an exchange spring

behavior: the soft YFe₂ layers reverse for positive bias fields, then, the irreversible switch of the hard DyFe₂ layers follows [17–19].

4. Influence of the temperature on the reversal process

The study of the influence of the temperature shows that the reversal may evolve, for a same sample, from a Soft layer First (SF) mechanism below 100 K to a Hard layer First (HF) above 100 K. In that case, the thermal energy may overcome the magnetic energy of the DyFe₂ layers; thus, it becomes easier to reverse the hard DyFe₂ layers for positive fields while the dominant magnetization of the soft YFe₂ layers remains aligned along the field. This result has been numerically evidenced with the DyFe₂ (5.5 nm)/YFe₂ (22 nm) multilayers for which the typical hysteresis loops are shown at $T=10$ K and $T=300$ K (Fig. 6(1) and (2)) and the coercive field B_c has been measured in function of the temperature (Fig. 6(3)).

The same typical results have been observed experimentally with the same layers' thicknesses [6]. The magnetization reversal has then been characterized by the measurement of the magnetic

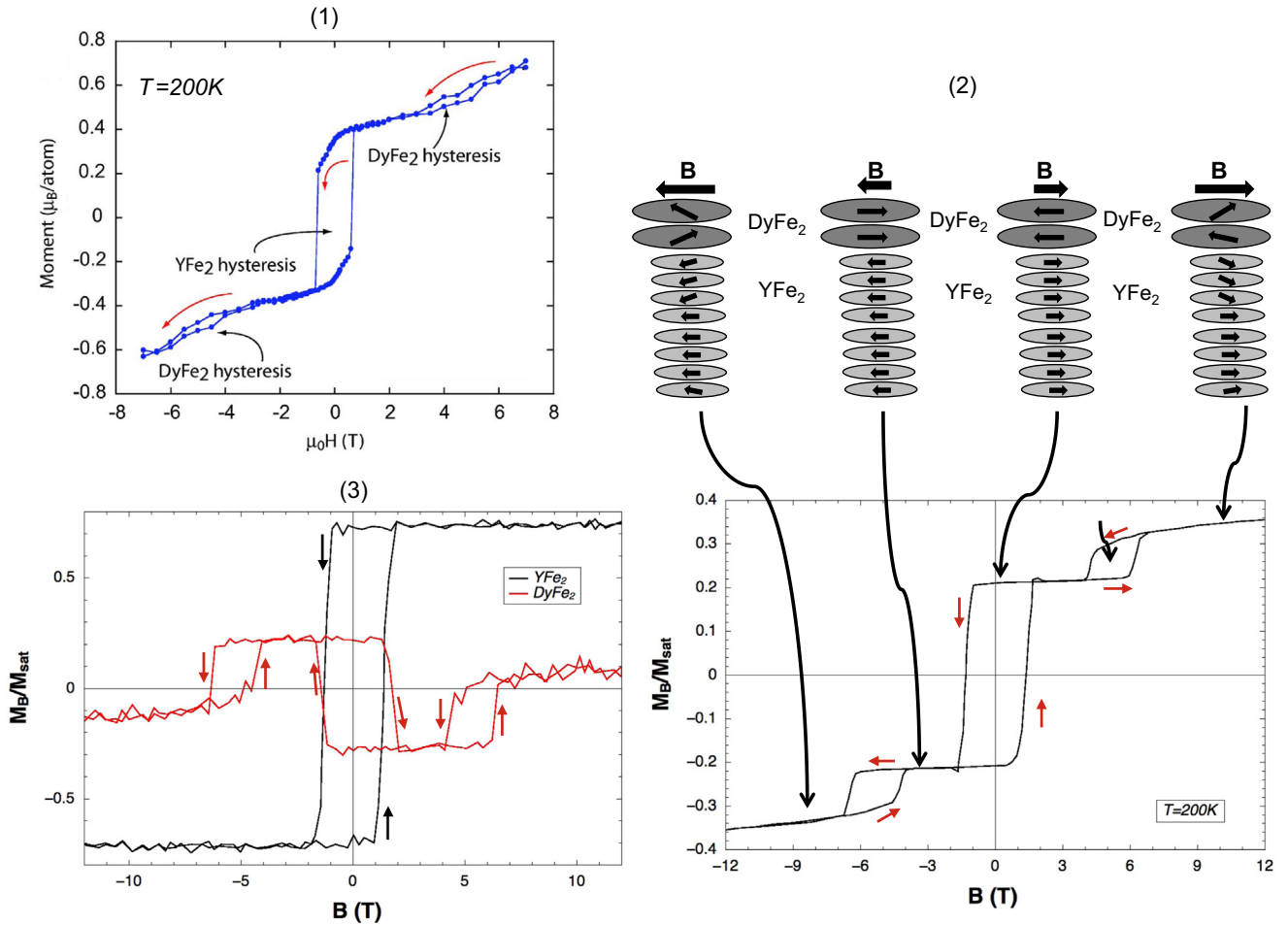


Fig. 4. Experimental (1) and simulated (2) hysteresis loops of DyFe₂ (3.2 nm)/YFe₂ (11.7 nm) superlattices showing a Hard layer First reversal [17]. The magnetization of the hard DyFe₂ and soft YFe₂ layers by Monte Carlo simulations which allows us to describe the reversal process of the DyFe₂ layers in three steps is also shown (3).

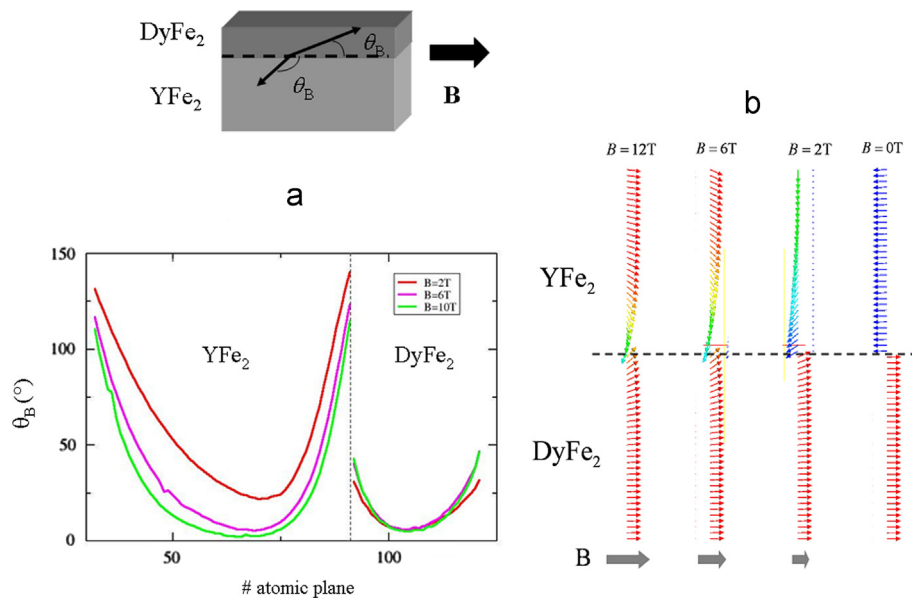


Fig. 5. (a) Evolution of the angle between the magnetization of each atomic plane and the magnetic field in function of the depth of the multilayer for different values of the magnetic field for the superlattice DyFe₂ (10 nm)/YFe₂ (20 nm). (b) Magnetization depth profile for different values of the decreasing magnetic field. In this representation, one bilayer only has been simulated which explains the fact that the symmetry is not reproduced (the configurations at the top and bottom of each layer are not the same).

field (H_Y) for which the YFe₂ magnetization reverses. This quantity, calculated in function of the temperature, allows us to determine 3 different temperature ranges: a “SF” region below 150 K, an “HF”

region above 200 K and an “intermediate” case between 150 and 200 K where both compounds are involved in the first step of reversal.

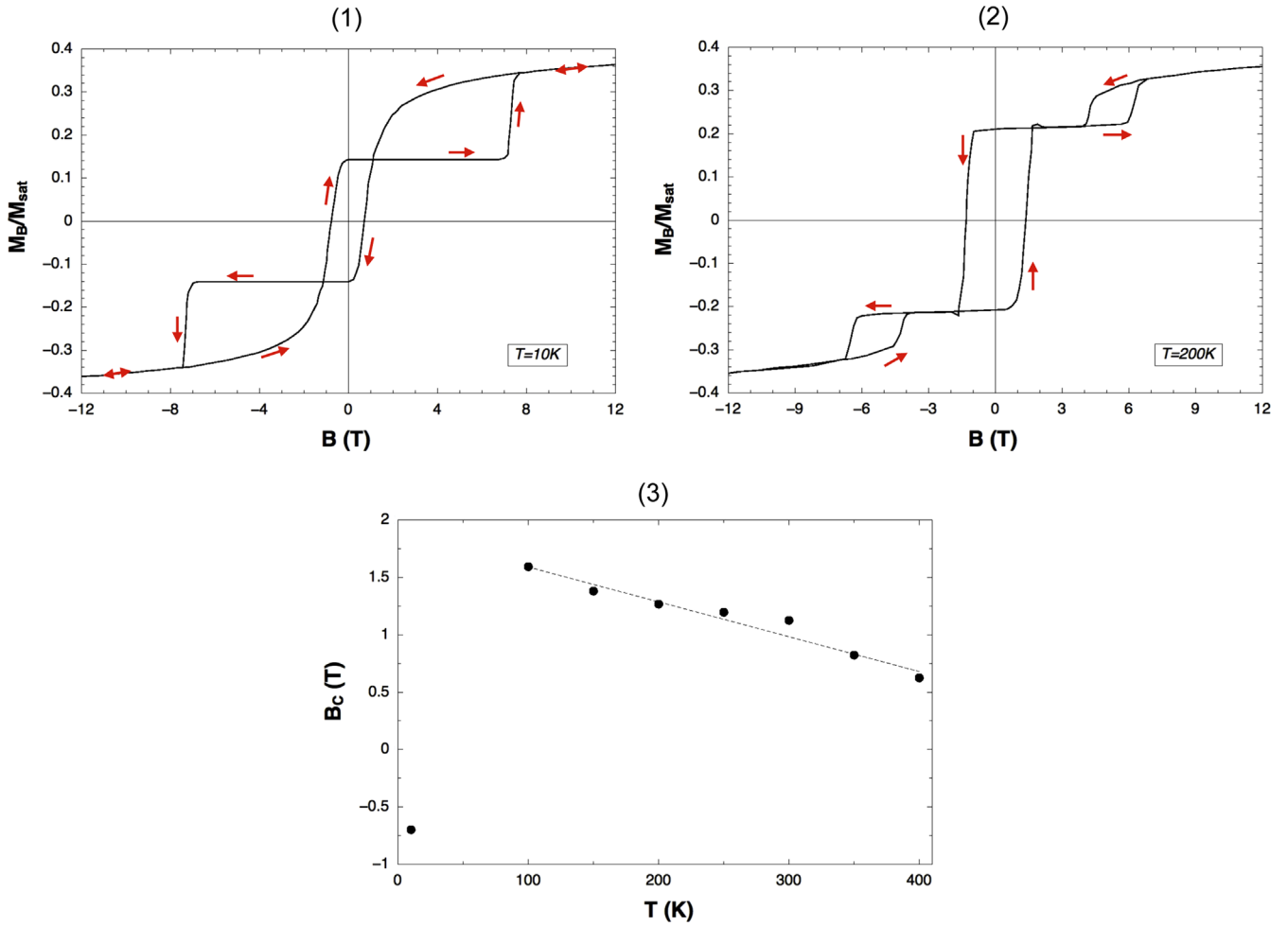


Fig. 6. Simulated hysteresis loops of DyFe_2 (5.5 nm)/ YFe_2 (22 nm) superlattices at $T=10\text{K}$ (1) and 300K (2) which evidences the strong variation of the coercive field B_c in function of the temperature (3).

It has also to be mentioned that micromagnetic simulations have been performed [10] which qualitatively reproduce the existence of two temperature regimes with the hard DyFe_2 layers switching at finite high temperature.

5. Conclusion

In this paper, 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 the switching of the magnetization in $\text{DyFe}_2/\text{YFe}_2$ multilayers. In particular, we have been able to reproduce hysteresis loops with characteristics matching those of experimental works at different temperatures. A strong temperature dependence of the magnetization reversal plays a key role for the reversal processes, and the interplay with exchange and Zeeman energy is understood on a qualitative level. The variation of the coercive field in function of the temperature, which depends not only on the soft/hard layers thicknesses ratio but also on the individual thicknesses, is due to the thermal change of the magnetic dominant configuration. The results of this study are in qualitative very good agreement with a great number of experimental works.

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