1. Introduction

Although the first clues about the interaction between an antiferromagnet (AFM) and a ferromagnet (FM) were already found 60 years ago with the discovery of exchange bias by Meiklejohn and Bean [1], still, not all of the details are fully understood today. The shift of the hysteresis loop when a FM/AFM bilayer is cooled in an external field below the Néel temperature $T_N$ and the increased coercivity of the loop were explained by considering uncompensated AFM spins at the interface, i.e. only one of the AFM sublattices couples to the FM. Theoretical calculations have shown that the surface energy density $J_I$ of this interface interaction is one or two orders of magnitude larger than the experimentally measured value [2]. This led to the conclusion that only a small fraction of the interfacial AFM spins contribute to the exchange bias in most systems. The other spins do not couple or rotate together with the FM, due to a locally reduced anisotropy or a stronger interfacial coupling [3].

Besides an increase in coercivity and a shift of the hysteresis loop, in most polycrystalline bilayers a training effect can also be observed, i.e. the bias field $B_{eb}$ and the coercivity $B_c$ decrease for an increasing number of hysteresis cycles $n$. This training effect can have two contributions: thermal and athermal training. Thermal training, which is generally much smaller than athermal training, happens for $n \geq 1$ and is rather well understood. Thermal fluctuations lead to a depinning of the frozen uncompensated spins at the interface and thus to a decrease in the bias field. The theory [4] shows that thermal training follows a power law given by $B_{eb}(n) \propto \frac{1}{\sqrt{n}}$, which has been confirmed extensively by experimental data [5–7]. Athermal training predominantly happens in the first hysteresis loop and often leads to an asymmetry in the first reversal of the FM towards negative saturation. It results from the frustrated metastable state of rotatable AFM spins after field cooling.

In a previous paper [8], we have shown that we were able to model the exchange bias and training effects, due to frozen and rotatable uncompensated AFM spins using MuMax3 [9], which is an open source micromagnetic simulation package that was primarily designed to study static and dynamic effects in ferromagnets. This GPU-accelerated software also allows for an easy implementation of the microstructure, e.g. to divide a micrometer sized sample into small grains by using a Voronoi tessellation [10].

When most of the AFM spins at the interface are compensated, i.e. if both sublattices of the AFM couple equally to the...
FM layer, the magnetic system will try to minimize its total energy by canting the AFM spins towards the FM [11–13]. This second order magnetic interaction [14], called spin flop coupling, produces a small net magnetic moment in the AFM and an increased coercivity [15]. Micromagnetic simulations [15] and theoretical considerations have shown, however, that, for an AFM with uniaxial anisotropy, this does not lead to exchange bias. Although the origin of this spin flop coupling is well understood, there are still a lot of unanswered questions, e.g. how is this increase in coercivity related to fundamental parameters and how and when can training effects result from compensated AFM spins?

In this paper, we will demonstrate how we can model spin flop coupling and training effects of a compensated AFM interface using MuMax3. In the next section, we will consider a simple model of an AFM with a strong uniaxial anisotropy and show that for small canting angles, spin flop coupling can be included by adding a custom energy density term \( \epsilon_{\text{sf}} \) and a custom field term \( \vec{B}_{\text{sf}} \) in MuMax3. Although this implementation is very efficient as only the ferromagnet needs to be taken into account, it has several drawbacks, e.g. these approximations are no longer valid for strong coupling parameters \( J_1 \) and training effects cannot be produced using this approach.

In the third section, we will show how MuMax3 can also simulate large canting angles by modelling a compensated AFM interface, consisting of two atomic AFM sublattices, by adding two extra layers in the micromagnetic model. Finally, the influence of spin flop coupling on the Landau state in square magnetic nanostructures will be compared to the experimental data and the case of training effects in an AFM with biaxial anisotropy will be discussed.

Having already shown that we can model uncompensated spins in a previous paper [8], we are now able to demonstrate for the first time how a mixed interface, containing compensated, as well as uncompensated, AFM spins, can be taken into account in one micromagnetic model. In this way, we can offer a good description of the static effects, due to the interface coupling between a FM and an AFM. Also, the coupling between synthetic antiferromagnets [16] and a FM layer can be modelled using this approach.

2. Spin flop coupling for small canting angles

As a toy model to describe spin flop coupling with a uniaxial AFM, we follow the macrospin approach where each magnetic subsystem (e.g. the FM and AFM sublattices) is assumed to be in a uniform state and can be described by a single magnetization vector.

We consider an infinite in-plane magnetized FM film (with thickness \( t_{\text{FM}} \) and saturation magnetization \( M_{\text{FM}} \)) coupled to a compensated antiferromagnet. The total surface energy density \( \sigma \) of this system can be written as

\[
\sigma = -\mu_0 M_{\text{FM}} t_{\text{FM}} H_{\text{ext}} \cos(\gamma - \beta) + \epsilon_K(\beta) t_{\text{FM}} + \sigma_{\text{AFM}} (\beta, \phi, \theta)
\]

where the function \( \epsilon_K(\beta) \) represents the anisotropy energy density of the FM and \( \beta \) and \( \gamma \) denote the angles that the FM and the external field \( H_{\text{ext}} \) make with the AFM anisotropy axis, respectively. We assume that the FM has a uniform uniaxial anisotropy perpendicular to the Néel axis, so \( \epsilon_K(\beta) = K_{\text{FM}} \cos^2(\beta) \). The function \( \sigma_{\text{AFM}}(\beta, \phi, \theta) \), which describes the interaction of the AFM (total thickness \( t_{\text{AFM}} \)) with the FM and the internal interaction between the AFM macrospins, is given by

\[
\sigma_{\text{AFM}}(\beta, \phi, \theta) = -J_1 \cos(\beta - \theta) + J_1 \cos(\beta + \phi) - K_{\text{AFM}} t_{\text{AFM}} \left[ \cos^2(\theta) + \cos^2(\phi) \right] - \delta t_{\text{AFM}} \cos(\theta + \phi)
\]

(2)

where \( J_1 \) is the coupling constant (surface energy density) between the FM and an AFM macrospin, \( K_{\text{AFM}} \) is the anisotropy constant of a sublattice and \( \delta \) the energy density linked to the mutual interaction between the two AFM sublattices. The definition of the angles \( \phi \) and \( \theta \), which the two AFM macrospins make with their anisotropy axes, is shown in figure 1.

As only the term \( \sigma_{\text{AFM}} \) in \( \sigma \) depends on the angles \( \phi \) and \( \theta \), it suffices to calculate the derivatives of \( \sigma_{\text{AFM}} \) towards \( \phi \) and \( \theta \) in order to minimize the total energy of the AFM. This leads to equations for \( \theta \) and \( \phi \) as a function of the angle \( \beta \). Assuming small canting angles, we can expand the function \( \sigma_{\text{AFM}} \) up to second order in \( \theta \) and \( \phi \), and so we can approximate the AFM energy density as

\[
\sigma_{\text{AFM}} \approx -J_1 \left[ \left( 1 - \frac{\phi^2}{2} \right) \cos(\beta) + \theta \sin(\beta) \right] + J_1 \left[ \left( 1 - \frac{\phi^2}{2} \right) \cos(\beta) - \phi \sin(\beta) \right] + K_{\text{AFM}} t_{\text{AFM}} \left[ \theta^2 + \phi^2 + \frac{\delta t_{\text{AFM}}}{2} (\theta + \phi)^2 \right]
\]

(3)

leaving out constant energy terms. Minimizing this energy density by calculating \( \frac{\partial \sigma_{\text{AFM}}}{\partial \theta} \) and \( \frac{\partial \sigma_{\text{AFM}}}{\partial \phi} \), we find an expression for \( \theta \) and \( \phi \) as a function of the FM angle \( \beta \).
\[
\begin{align*}
\theta(\beta) &= \frac{J_1 \sin(\beta) [-J_1 \cos(\beta) + 2K_{AFM} \cos(\beta)]}{4t_{AFM}^2 K_{AFM} (K_{AFM} + \delta) - J_1^2 \cos^2(\beta)} \quad (4) \\
\phi(\beta) &= \frac{J_1 \sin(\beta) [J_1 \cos(\beta) + 2K_{AFM} \cos(\beta)]}{4t_{AFM}^2 K_{AFM} (K_{AFM} + \delta) - J_1^2 \cos^2(\beta)}.
\end{align*}
\]

These two equations show that for \( \beta = \frac{\pi}{2} \) the angles of the AFM macrospins are symmetrical around the FM direction \( \beta \), i.e. \( \theta = \phi \). After substituting these angles \( \theta(\beta) \) and \( \phi(\beta) \), which minimize the AFM energy density \( \sigma_{AFM} \), in equation (3), we find that

\[
\sigma_{AFM}(\beta) \approx -\frac{\kappa \sin^2(\beta)}{1 - \frac{2K_{AFM}^2}{\sigma_{AFM}^2}} \quad (6)
\]

where we have defined the constant \( \kappa = \frac{t_{AFM}^2 K_{AFM}}{K_{AFM} + \delta} \).

Retaining only the lowest order approximation in \( \frac{1}{\sigma_{AFM}^2} \) in the case of low coupling, one finally obtains that

\[
\sigma_{AFM}(\beta) \approx \kappa \cos^2(\beta). \quad (7)
\]

This equation describes the spin flop coupling for small canting angles, i.e. the energy of the antiferromagnet is minimal when the ferromagnet is perpendicular \( (\beta = \frac{\pi}{2}) \) to the AFM Néel vector and so in this case \( \theta = \phi = \frac{\pi}{2} \).

The total surface energy density can then be written as

\[
\sigma = -\mu_0 M_{FM} H_{ext} \cos(\gamma - \beta) + \frac{K_{AFM} H_{FM} + \kappa}{2} \cos^2(\beta)
\]

and the switching field \( B_c \) for \( \gamma = \frac{\pi}{2} \) is given by

\[
B_c = \frac{2}{M_{FM}} \left[ K_{FM} + \frac{J_1^2}{2t_{AFM}^2 K_{AFM} (K_{AFM} + \delta)} \right]. \quad (9)
\]

This shows that spin flop coupling only leads to a renormalization of the uniaxial anisotropy constant \( K_{FM} \) and thus to an enhanced coercivity for a hysteresis loop measured perpendicular to the Néel vector of the AFM.

Given the parameters \( J_1, K_{AFM} \) and \( \delta \), one can implement spin flop coupling in MuMax³ by adding a constant energy density \( \epsilon_{df} \) and a corresponding effective field \( \vec{B}_{df} \), defined as

\[
\epsilon_{df} := - \frac{1}{2} M_{FM} \cdot \vec{B}_{df} = \frac{\kappa}{K_{FM}} \cos^2(\beta) \quad (10)
\]

\[
\vec{B}_{df} = - \frac{2\kappa}{M_{FM} H_{FM}} (\vec{u} \cdot \vec{m}) \vec{u}
\]

with \( \vec{m} \) being the normalized magnetization vector of the FM and \( \vec{u} \) the Néel vector, i.e. the anisotropy direction of the AFM. As expected, this spin flop model does not produce exchange bias.

In case the two AFM macrospins couple with different strengths to the FM, one can approximate the exact energy terms again for small canting angles and show that this leads to exchange bias as a first order effect, given by

\[
\sigma_{AFM}(\beta) = - [J_{L,\theta} - J_{L,\phi}] \cos(\beta).
\]

3. Full micromagnetic description of spin flop coupling

3.1. Micromagnetic model

In a micromagnetic approach, the atomic magnetic moments and their quantum mechanical interactions are averaged over a nanometer length scale, which is sufficiently small to resolve magnetic structures like domain walls. This approach has been used for many years to model ferromagnets, where the exchange interaction does not allow for sharp changes in the magnetization. In an AFM where the magnetic moments alternate direction on consecutive atomic sites, this approach would result in a zero net magnetization. However, at the micromagnetic scale, the two atomic sublattices of an AFM can be considered as two separate, smoothly varying ferromagnetically ordered lattices, which are antiferromagnetically coupled and coincide in space.

Disregarding the atomic scale of these sublattices means that the dynamics relevant on this length scale (e.g. AFM spin waves) are lost, just like the high frequency part of the spin wave spectrum is also lost in a FM model when the local variations are averaged out. However, the static interaction between the two sublattices is not lost, as the exchange interaction between the sublattices is taken into account in the micromagnetic model.

For interfaces with thin FM and AFM layers, single micromagnetic layers can be used. As a micromagnetic cell can only contain one magnetization vector in MuMax³, the coinciding cells of an AFM layer are separated into two different layers, denoted AFM1 and AFM2 (see figure 2). This separation in space has no physical implications. Even though the AFM1 layer (figure 2) is not directly adjacent to the FM layer, a direct coupling can be established by adding a custom field and energy term (see supplementary material (stacks.iop.org/JPhysD/50/425002/mmedia)). A negative interlayer exchange stiffness \( A_{AFM} \) will ensure the antiferromagnetic coupling of the sublattices and a positive intralayer exchange stiffness \( A_{A} \) of the same magnitude will allow for the correct domain wall energy in the AFM (see the supplementary material).
3.2. Limitations of the model

Due to the micromagnetic approximation of the AFM and its implementation in MuMax\(^3\), no high frequency dynamics due to the exchange interaction between the two AFM sublattices can be modelled in our simulations. When studying quasi-static configurations resulting from an energy minimisation, precession does not have to be taken into account. This is the case for the problems studied in this paper: exchange bias, spin flop coupling and athermal training.

In case of a thicker antiferromagnet, one can expect that the bulk AFM spins will be pinned along the anisotropy axis and only the AFM spins at the interface region will cant towards the FM. As introduced in the model of Mauri [17], a planar domain wall can form, which can be included by adding a third fixed layer\(^1\) or by subdividing the AFM into several bilayers.

3.3. Implementation

As discussed in section 3.1, each AFM layer can be modelled as a pseudo-ferromagnetic layer with thickness \(t_{\text{AFM}}\) and anisotropy constant \(K_{\text{AFM}}\). The interfacial exchange energy \(J_I\) and the energy density \(\delta\) linked to the mutual interaction between the two AFM spins can be defined in terms of exchange stiffnesses between the FM/AFM and the two AFM layers, respectively. Using the convention used in MuMax\(^3\) for the exchange energy density, one obtains that \(A_I = \frac{J_I}{C}\) and \(A_{\text{AFM}} = -\frac{2 \delta_{\text{AFM}} C}{S}\) with \(C\) the cell size perpendicular to the interface. Assuming that a micromagnetic system consists of two AFM sublattices and one FM layer, one can couple the FM layer with the nearest AFM layer (AFM\(_2\) in figure 2) by rescaling the exchange stiffness using the scaling factor \(S\) as defined in [9] and discussed in the supplementary material. As in the standard version of MuMax\(^3\), only the nearest neighbouring cells are taken into account for the evaluation of the exchange energy, one has to couple the other AFM layer, labelled by AFM\(_1\) in figure 2, with the FM layer by using periodic boundary conditions, perpendicular to the FM/AFM interface or by defining a custom field/energy term. The former approach can only be used when the FM consists of only one layer, while the addition of a custom field/energy term is generally applicable. Demagnetization energy should be turned off in the AFM layers and care should be taken when defining the saturation magnetization \(M_{\text{AFM}}\) in the antiferromagnet. For more information, see the supplementary material.

It is important to note that one can take into account the compensated as well as uncompensated (rotatable as well as pinned) AFM spins in the same micromagnetic simulation using this approach. It suffices to locally decouple one AFM layer of the FM and locally set \(\delta = 0\). In this case, the sublattice anisotropy constant \(K_{\text{AFM}}\) has to be replaced by the total anisotropy constant of the antiferromagnet.

\(^1\)In this case one has to add an energy term \(-J_I \cos(\phi) - J_o \cos(\theta)\) in the macrospin model (equation (2)). The parameter \(J_o\) is the surface energy density to form a planar domain wall in the antiferromagnet.

\(^2\)In the simulations \(H_{\text{ext}}\) is set at a small angle of 1° with the defined directions to introduce a slight asymmetry.

Figure 3. Coercivity \(B_c\) as a function of the coupling constant \(J_I\). The small canting angle approximation (red curve) is valid up to \(J_I \approx 2 \text{ mJ m}^{-2}\). The breakdown of the canted spin flop state happens around \(J_I \approx 4.5 \text{ mJ m}^{-2}\) and leads to a vanishing coercivity for a hysteresis loop measured perpendicular (green curve) to the Néel vector. The blue curve is the coercivity of a hysteresis loop measured parallel to the Néel vector.

3.4. Breakdown of the small canting angle approximation

To compare the coercivity \(B_c\) derived from the small canting angle approximation (equation (9)) with the coercivity resulting from the exact energy terms, a simple system was studied with \(t_{\text{AFM}} = t_{\text{FM}} = 3 \text{ nm}, M_{\text{FM}} = 1400 \text{ kA m}^{-1}, \delta = 1 \times 10^6 \text{ J m}^{-3}\) and \(K_{\text{AFM}} = 7 \times 10^5 \text{ J m}^{-3}\). Demagnetization energy was turned off in the FM and no FM anisotropy was considered. To avoid metastable states, each simulation consisted of two consecutive hysteresis loops for \(H_{\text{ext}}\) parallel\(^2\) and perpendicular to the uniaxial anisotropy axis of the AFM. The coercivity of the second hysteresis loop together with the small canting angle approximation reported in the previous section are shown in figure 3.

One can see that, for these parameters, the small angle approximation of our model is valid up to \(J_I \approx 2 \text{ mJ m}^{-2}\) where the relative error is around 5%. In figure 4, the minimized total surface energy density (without Zeeman energy) of the system is shown as a function of the angle \(\beta\) for different coupling constants \(J_I\).

For low \(J_I\), the minima are located at the angles \(\beta = \pm \frac{\pi}{2}\), representing the global energy minima. This corresponds to what was discussed in the small canting angle approximation, as can be seen in equation (10). Even though the approximation is not valid anymore around \(J_I \approx 2 \text{ mJ m}^{-2}\), the spin flop state is still the global energy minimum and will lead to a vanishing coercivity for a hysteresis loop, measured parallel to the AFM easy axis, as can be seen in figure 3.

At \(J_I \approx 4.5 \text{ mJ m}^{-2}\) however, the shape of the energy function changes because the canted spin flop state is not the global energy minimum anymore as a spin flip transition occurs, similarly to the metamagnetic spin flip transition of an antiferromagnet in a strong magnetic field. In this case, the interface coupling \(J_I\) overcomes the intersublattice interaction
nel vector in figure 3 and a vanishing coercivity at leads to a finite coercivity in the hysteresis loop parallel to the nel vector becomes a hard axis. This i.e. parallel to the easy axes of the AFM, and the direction resulting in a parallel orientation of the two AFM layers. For a rescaling of the AFM parameters to achieve the correct total energy, please see the supplementary material.

3.5. Interface coupling in LSMO/LFO square nanostructures

As a first application of our micromagnetic model for spin flop coupling, we reproduce the experimental X-PEEM data of epitaxially grown La$_{0.7}$Sr$_{0.3}$MnO$_3$(35 nm)/compensated LaFeO$_3$(3.8 nm) square nanostructures as has been reported by Takamura et al in [18]. They noticed that in the bilayer, the Néel vector of the antiferromagnetic LFO was oriented perpendicular to the domain structure in the ferromagnetic LSMO square, in accordance with spin flop coupling between the FM and compensated AFM.

Two types of FM domain structures were observed in the LSMO/LFO squares. The authors argued that these structures result from variations in the local bias field, induced by the DMI interaction. For low bias fields, a Landau structure (with a displaced vortex) is found while higher local bias fields result in a z-type domain. A corresponding perpendicular domain structure was found in the AFM. For a single uncoupled LSMO layer, only the typical Landau domain structure was observed. This implies that variations of the local bias field could change the domain structure of the LSMO layer and thus also of the AFM.

The ferromagnetic LSMO has biaxial anisotropy with two easy axes, denoted by the vectors $\vec{c}_1$ and $\vec{c}_2$, oriented along the (110) directions, i.e. the sides of the $2 \times 2 \mu m^2$ square. The anisotropy energy density is given by $\epsilon_K = K_c (\vec{c}_1 \cdot \hat{m})^2 (\vec{c}_2 \cdot \hat{m})^2$ with $\vec{c}_1$ pointing along the $x$-axis and $\vec{c}_2$ along the $y$-axis of the simulation box. The bilayer was divided into $512 \times 512 \times 2$ AFM + 1 FM cells with a lateral cell size of 3.9 nm and thickness of 35 nm. For the ferromagnetic LSMO, we used typical parameters: $M_{FM} = 400 \kappa A m^{-1}$, $A_{FM} = 1.8 \mu J m^{-1}$ and $K_{c,FM} = 1.6 kJ m^{-3}$.

Experiments [18, 19] show that 60% of the AFM domains in the LFO layer have their biaxial easy axes along the (110) directions and the remaining 40% have their easy axes along the (100) directions. Therefore, the anisotropy axes were distributed accordingly for the AFM layer in our simulations by using a Voronoi tessellation. We used the parameters: $\delta = 1.25 \times 10^3 J m^{-3}$, $K_{c,AFM} = 1.5 kJ m^{-3}$ and $J_I = 0.17 mJ m^{-2}$ for the interaction between the AFM and FM.

Starting from a random FM state and semi-random AFM state, the system was relaxed towards equilibrium after being subjected to thermal fluctuations (70 K during 0.2 $\mu$s). The FM and the average of the absolute value of the magnetisation of the two AFM layers (at remanence) are shown in figure 5.

In this case, the AFM orients itself perpendicular to the FM as the ferromagnetic domain structure is determined by the demagnetisation energy. A similar effect was also observed in NiO/Fe and CoO/Fe nanodisks [20].

In the experimental data shown in figure 3 of [18], however, z-type of domains in the FM and corresponding perpendicularly coupled domains in the AFM were also found. By comparing the data to a micromagnetic simulation of only the FM layer, the authors state that these domain structures appear for bias fields above a threshold of approximately 9 mT and correspond to a vortex, displaced towards the corner of a square. To test this hypothesis, a hysteresis loop of the FM/compensated AFM square was simulated with an external field, representing the bias field $B_b$, applied along one of the diagonals. Starting from remanence, as shown in figure 5, the flux closed vortex state is stable for $B_b \leq 8$ mT. For a bias field of 8 mT, the vortex gets displaced towards the corner of the square. For $B_b > 8$ mT, z-domains are formed in the FM and a corresponding perpendicular domain structure is found by the strong magnetocrystalline anisotropy of the AFM, the global energy minimum anymore. Each curve was shifted by $\delta = \delta_1 - \delta_2 = 2\pi J \mu m^2$.

Figure 4. Minimal surface energy density curves $\sigma$ as a function of the FM rotation angle $\beta$. A spin flip transition happens for $J_I \approx 4.5 mJ m^{-2}$, which leads to the fact that the spin flop state is not the global energy minimum anymore. Each curve was shifted by $\sigma(\beta = 0^\circ)$. The values of the curve for $J_I = 5 mJ m^{-2}$ correspond to the scale on the right.

Figure 5. Spin flop coupling in a LSMO/LFO nanosquare for $B_b = 0$ mT, initialized from a random state. (a) The typical Landau domain structure in the ferromagnetic LSMO. (b) The average of the absolute values of the magnetization of the two antiferromagnetic LFO layers. (c) The color scale of the magnetization. The magnetization vector is tangent to the circle shown.

$\delta$ resulting in a parallel orientation of the two AFM layers. Due to the strong magnetocrystalline anisotropy of the AFM, the global energy minima are now given by $\beta = 0$ and $\pi$, i.e. parallel to the easy axes of the AFM, and the direction perpendicular to the Néel vector becomes a hard axis. This leads to a finite coercivity in the hysteresis loop parallel to the Néel vector in figure 3 and a vanishing coercivity at the scale on the right. 

5 30% of the AFM grains were initialised along the $x$-axis, 30% along the $y$-axis, 20% along one diagonal of the square and 20% along the other diagonal. The sublattices were initialised each time antiparallel to each other. 

6 See figures 4(c) and (d) in [18].

7 When the LSMO is not coupled to the LFO, no bias field can be present and thus only Landau states are formed in the ferromagnet.
in the AFM layers\textsuperscript{8}. These three magnetic configurations are shown in figure 6.

When returning from saturation, however, the FM does not return towards the vortex state for $B_b < 8$ mT. The presumption thus arises that these z-domains can also be present in lower bias fields, as opposed to what was claimed by the authors in [18]. When initializing the FM from completely random states, only Landau domain structures were found for $B_b = 0$ mT. Relaxing different random states in a bias field $B_b = 5$ mT, z-domains, as well as domains with a displaced vortex, were formed. The results are shown in figure 7. Note that two variations of the z-domain can be found due to the symmetry of the system, in correspondence to the experimental data. When $B_b \geq 7.5$ mT only z-domains were formed. This shows that the creation of z-domains are indeed

\textsuperscript{8}The domain wall in the AFM is induced by the initial Landau state.

3.6. Athermal training effects

3.6.1. Hoffmann training. As a second example, we will take a look at the training effect in a compensated AFM, as was proposed by Hoffmann [21] and is nowadays generally accepted [22, 23]. While there can be no training effects or exchange bias in a perfectly compensated antiferromagnet with uniaxial anisotropy, Hoffmann argued that this is not the case when the AFM has a fourfold (or higher) magnetocrystalline anisotropy. He argued that, after field cooling, the sublattices of the AFM can be in a non collinear state and only relax towards an antiparallel configuration after the first reversal of the FM. This produces an athermal training effect and exchange bias in the first hysteresis loop ($n = 1$). Also, the asymmetry between the first drop in the hysteresis loop and its reversal towards positive saturation is a prominent feature of athermal training.

3.6.2. Phase diagram of Hoffmann training. As the training effect in the model of Hoffmann results from a non collinear state of the two AFM sublattices induced by field cooling, we can expect that training will only happen within a certain parameter range. As an example, we will investigate this effect by considering a uniform biaxial compensated antiferromagnet whose easy axes make an angle of 45° with respect to the field cooling direction. To simulate field cooling, the AFM layers were initialized in a spin flop state, i.e. in the (1 1 0) and (1 − 10) directions along their easy axes. Afterwards the system was relaxed while the FM was saturated in the field cooling direction. A cell size of 2 nm in the in-plane direction and a cell thickness of 10 nm was chosen in a direction perpendicular to the interface, i.e. in this case $t_{FM} = t_{AFM} = 10$ nm. For the FM typical parameters of Py were used: $M_{FM} = 800$ kA m$^{-1}$, $A_{FM} = 13$ pJ m$^{-1}$ and magnetocrystalline anisotropy was not

\textsuperscript{9}$H_{ex}$ is set at a small angle of 1° with the field cooling direction to introduce a slight asymmetry.
considered. For the antiferromagnet we used $\delta = 8 \times 10^4$ J m$^{-3}$. The biaxial anisotropy constant $K_{\text{AFM}}$ and the coupling parameter $J_I$ were varied and the coercivity and exchange bias field were determined for two consecutive hysteresis loops along the field cooling direction. The Zeeman energy was not taken into account for the AFM.

The result of this parameter scan is shown in figure 8 where the difference in coercivity between the first and second hysteresis loop is displayed. Reduced dimensionless units were used, i.e.

$$j = \frac{J_I}{\delta_{\text{AFM}}} \quad k = \frac{K_{\text{AFM}}/\delta_{\text{AFM}}}{\delta_{\text{AFM}}} \quad h_c = \frac{\mu_0 M_{\text{FM}} H_c}{\delta_{\text{AFM}}}$$

for the interface coupling, anisotropy and coercivity, respectively. The different reversal mechanisms, present in the phase diagram, are illustrated in figure 9 for a coupling constant of $j = 1.75$.

One can clearly distinguish two regions displaying training effects in the phase diagram. The middle region is the real Hoffmann training (figure 9(c)) as explained in the previous section: the AFM layers change from a non collinear to an almost antiparallel arrangement after the first drop in the hysteresis loop. After this irreversible transition, the AFM layers will induce spin flop coupling (see supplementary material) in the FM layer, but with an easy axis rotated over 45° with respect to the field cooling direction. According to the Stoner Wohlfarth model, they will also contribute to the coercivity in the second hysteresis loop, but its value will be reduced by a factor of 2. The coercivity $h_{c,2}$ of the second hysteresis loop (after training) for $j = 1$ as a function of the reduced anisotropy constant $k$ can be seen in figure 10. Hoffmann training is present from $k \approx 0.75$ to $k \approx 3.5$. The rise in coercivity for $k < 0.75$ is due to the fact that both AFM layers are approximately in a 90° canted position and switch together with the FM. For this configuration (figure 9(a)), an increasing anisotropy constant leads to an increasing coercivity, in contrast to the case of spin flop coupling.

The training effect in the lower right part (high coupling and low anisotropy) of the phase diagram (figure 8) is the result of a spin flip transition. After reaching negative saturation in the first hysteresis loop, the two AFM layers stay parallel to each other in further hysteresis loops. This mechanism is shown in figure 9(b). A similar effect was already seen when considering the breakdown of the canted spin flop state for an AFM with uniaxial anisotropy (section 3.4). In this case, the AFM layers switch irreversibly with the FM for $n > 1$, which leads to a higher coercivity. This is not the case for Hoffmann training. Both regions in the phase diagram, however, display the asymmetry in the first hysteresis loop, which is typical for athermal training, as can be seen in figure 11.
Athermal training also leads to exchange bias in the first hysteresis loop, due to a change in coercivity. For high anisotropy constants $k$ and low coupling constants $j$, i.e. in the upper left part of the phase diagram, one can in fact obtain the exchange bias for $n \geq 1$ as the AFM spins are pinned in a spin flop state along the field cooling direction as displayed in figure 9(d). The phase diagram for exchange bias in the case $n \geq 1$ is shown in figure 12. Using the small angle approximation in an AFM with biaxial anisotropy, one can calculate (see the supplementary material) the bias field $B_{eb}$ for high anisotropy constants. In figure 13, one can see that there is a good agreement between this model and the values obtained from our simulations. Also the bias field for two fixed uncompensated spins, which make an angle of 45° with the field cooling direction, is shown as comparison (green line in figure 13). We remark that in an experiment, one cannot distinguish between a frozen uncompensated AFM spin or two compensated biaxial AFM spins, frozen into a 90° canted state, as both have the same net effect on the FM layer.

If one assumes a negative coupling constant $J_I$ and takes into account the Zeeman energy for the AFM, one can also obtain positive bias fields, similar to the model that was proposed by Kiwi [24]. For low cooling fields $H_{fc}$, the pinned compensated AFM spins will be antiparallel to the cooling field direction. For stronger cooling fields, however, the AFM spins can make an irreversible transition of 90° due to the Zeeman energy and produce a net magnetic moment parallel to $H_{fc}$. As hysteresis loops are often recorded for $H_{ext} \ll H_{fc}$, these spins stay pinned in the spin flop configuration due to the strong magnetocrystalline anisotropy and low coupling to the FM, even during reversal of the ferromagnet.

Additionally, a system with a polycrystalline biaxial AFM layer was simulated in the same parameter range as for the uniform case. For each parameter set, the same grains with the same anisotropy axes were used. The AFM intergrain interaction was not taken into account. The difference in coercivity between the first and second hysteresis loop is shown in figure 14. Apart from small fluctuations, the global shape of the phase diagram is very similar to figure 8. The distinct separation between the region of Hoffmann training and the spin flip arrangement is less clear due to the random distribution of the anisotropy axes. The bias field in the second hysteresis loop ($n = 2$) is shown in figure 15 and is also similar.
Figure 15. Exchange bias field $b_{ex}$ for $n = 2$ in a polycrystalline AFM for grains with biaxial anisotropy, as a function of the reduced anisotropy constant $k$ and the reduced exchange coupling $j$. The same parameters were used as in the uniform case shown in figure 8. The color scale is to the right.

Figure 16. Average behaviour of the two AFM layers ($j = 2$ and $k = 4,1$) at negative and positive saturation, labelled by (a) and (b) respectively. Note that the vectors shown only indicate the orientation of the average magnetizations of the AFM$_{1}$ and AFM$_{2}$ layers and not the magnitude. The angle the FM makes with respect to the external field is a bit exaggerated. The biaxial anisotropy axes (blue) are shown as a comparison.

to figure 12. In some regions there is still a non vanishing bias field for $n \geq 2$. The bias field in the region $j = 2$, $k = 4$ originates from the fact that the absolute value of the average $x$-component of the AFM$^{10}$ is asymmetric at positive and negative saturation. In the uniform case, we find $\langle m_{x,\text{AFM}} \rangle \approx 0.24$ and $\langle m_{x,\text{AFM}} \rangle \approx -0.24$ for positive saturation and negative saturation, respectively. In the polycrystalline case (figure 16), however, we retrieve that $\langle m_{x,\text{AFM}} \rangle \approx 0.03$ for negative saturation, but $\langle m_{x,\text{AFM}} \rangle \approx 0.41$ for positive saturation. As $\langle m_{x,\text{AFM}} \rangle > 0$ for positive as well as negative saturation, a net average torque is applied on the FM layer and thus exchange bias is produced. The average $y$-components are symmetric at positive and negative saturation, but with opposite signs. This asymmetry is induced by the finite number of AFM grains in our simulation box and by the fact that some AFM grains are in a frozen spin flip state in the direction of the cooling field after initialization, leading to a net preferred direction.

In the region $j = 2$, $k = 1.6$, a spin flip transition of the two AFM layers occurs, analogous to the uniform case. The moments of the two AFM layers inside an AFM grain will be parallel after the first reversal ($n = 1$) towards negative saturation. The total average $y$-component of the antiferromagnet are $\langle m_{y,\text{AFM}} \rangle \approx -0.12$ and $\langle m_{y,\text{AFM}} \rangle \approx -0.34$ at positive and negative saturation, respectively. The spin flip state together with the effect of the limited size also produces here a small exchange bias.

One can conclude that the average behaviour of a polycrystalline AFM is analogous to the case where the two biaxial anisotropy axes are set symmetrical along the field cooling direction.

3.6.3. Reproducing athermal training in an IrMn/CoFe bilayer. As an illustration of the implementation of mixed antiferromagnetic interfaces in MuMax$^{3}$ and training effects in a compensated AFM, we will reproduce the experimental hysteresis loop of an IrMn(15 nm)/CoFe(10 nm) bilayer, measured at 15 K, as was reported by Fulara et al$^{25}$ (see inset figure 1(b)). Although IrMn has uniaxial anisotropy at high temperatures, experimental evidence$^{25, 26}$ shows that the AFM undergoes a phase transition at 50 K and develops a biaxial anisotropy during field cooling. The observed training is attributed to Hoffmann training, as it does not follow the power law for thermal training.

The simulation box is divided into $512 \times 512 \times 2$ AFM$^{+1}$ FM cells of 3 nm lateral size and 10 nm in thickness. For the FM, typical parameters$^{27, 28}$ were used: $M_{FM} = 1600 \text{ kA m}^{-1}$ and $A_{FM} = 2.5 \times 10^{-11} \text{ J m}^{-1}$. A small uniaxial anisotropy ($K_{FM} = 4 \text{ kJ m}^{-3}$) was applied in the field cooling direction to model magnetic annealing. The antiferromagnetic IrMn was divided into 20 nm grains using a Voronoi tessellation with randomly distributed anisotropy axes. In the AFM, no intergrain interaction was taken into account. To simulate an infinite thin film, periodic boundary conditions were applied, using a macro geometry approach where five copies of the system were taken into account in the in-plane directions$^{9, 29}$.

The parameters$^{11}$ of the AFM layer were tuned in order to match the experimental hysteresis loop: $A_{\text{AFM}} = -1.88 \times 10^{-11} \text{ J m}^{-1}$, $A_{1} = 1.7 \times 10^{-11} \text{ J m}^{-1}$ and as biaxial anisotropy constant we used $K_{c,\text{AFM}} = 2.25 \times 10^{3} \text{ J m}^{-3}$.

$^{11}$For a rescaling of the AFM parameters to achieve the correct total energy, see the supplementary material.
Due to the definition of the biaxial anisotropy energy density, approximately 20% of the AFM spins were initialized into a 45° canting configuration with respect to the field cooling direction and 76% were randomly distributed, with antiparallel sublattices. In order to produce a small exchange bias, the two sublattices couple differently towards the ferromagnet or to cases where the antiferromagnet consists of three or to cases where the antiferromagnet consists of three uncompensated AFM spins, which are frozen anymore for $n > 1$.

As this is a reversible transition, no training effect is obtained anymore for $n > 1$.

In figure 19, one can see in which grains the two AFM layers are in a non collinear (red color) and antiparallel (blue color) state after field cooling and at negative saturation for $n = 1$. One can see that after the first drop in the hysteresis loop towards negative saturation, the two AFM layers are antiparallel in all grains, except in those of the pinned uncompensated AFM grains. For comparison, the case of a polycrystalline IrMn layer with uniaxial anisotropy is shown in figure 20. As expected, no training effect is found.

4. Conclusions

We have shown how to implement compensated antiferromagnetic interfaces to model hysteresis loops of ferromagnets using MuMax³. This can be achieved by either using the small canting approximation in the case of low coupling constants or by adding two extra AFM layers to the simulation box. By using the latter micromagnetic approach, we can not only reproduce athermal training effects or spin flop coupling, but we can also take into account compensated and uncompensated AFM spins in one micromagnetic simulation and therefore give a good description of realistic FM/AFM interfaces. By demonstrating this model, we have opened a door for new micromagnetic studies of complex AFM/FM interfaces with both compensated and uncompensated spins. Static problems, such as the stability of the FM domain configurations can be investigated. This implementation can easily be extended to antiferromagnets with higher symmetries, to cases where the two sublattices couple differently towards the ferromagnet or to cases where the antiferromagnet consists of three sublattices.

Approximately 20% of the AFM spins were initialized into a 45° canting configuration with respect to the field cooling direction and 76% were randomly distributed, with antiparallel sublattices. In order to produce a small exchange bias field for $n \geq 2$, about 4% pinned uncompensated spins were randomly added to the AFM layers, as discussed before (section 3.3). A quasistatic hysteresis loop was simulated along the field cooling direction. The result is shown in figure 17. One can clearly see the asymmetry and the reduction of the coercivity in the first hysteresis loop. During the hysteresis loop of the polycrystalline IrMn/CoFe bilayer, also the average behaviour of an AFM grain, whose easy axes $K_{\text{c,AFM}}$ make an angle of 45° with respect to the field cooling direction $f_c$. The two sublattices (red and green) relax from a non collinear to the positive saturation again.

As this is a reversible transition, no training effect is obtained anymore for $n > 1$.

In figure 19, one can see in which grains the two AFM layers are in a non collinear (red color) and antiparallel (blue color) state after field cooling and at negative saturation for $n = 1$. One can see that after the first drop in the hysteresis loop towards negative saturation, the two AFM layers are antiparallel in all grains, except in those of the pinned uncompensated AFM grains. For comparison, the case of a polycrystalline IrMn layer with uniaxial anisotropy is shown in figure 20. As expected, no training effect is found.

4. Conclusions
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