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Charilaou, M

Hellman, F

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Roughness effects in uncompensated antiferromagnets

M. Charilaou^{1,2,3,a)} and F. Hellman^{1,2}

¹*Department of Physics, University of California, Berkeley, California 94720, USA*

²*Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA*

³*Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, Zurich 8093, Switzerland*

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Monte Carlo simulations show that roughness in uncompensated antiferromagnets decreases not just the surface magnetization but also the net magnetization and particularly strongly affects the temperature dependence. In films with step-type roughness, each step creates a new compensation front that decreases the global net magnetization. The saturation magnetization decreases non-monotonically with increasing roughness and does not scale with the surface area. Roughness in the form of surface vacancies changes the temperature-dependence of the magnetization; when only one surface has vacancies, the saturation magnetization will decrease linearly with surface occupancy, whereas when both surfaces have vacancies, the magnetization is negative and exhibits a compensation point at finite temperature, which can be tuned by controlling the occupancy. Roughness also affects the spin-texture of the surfaces due to long-range dipolar interactions and generates non-collinear spin configurations that could be used in devices to produce locally modified exchange bias. These results explain the strongly reduced magnetization found in magnetometry experiments and furthers our understanding of the temperature-dependence of exchange bias. © 2015 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4913594>]

I. INTRODUCTION

Antiferromagnets (AFM) are materials in which the atomic spins couple antiparallel to each other thus compensating one another, seemingly resulting in zero magnetization for an infinite perfect crystal. Defects and surfaces however introduce the possibility of uncompensated moments. In particular, surfaces can lead to a symmetry-breaking net magnetization $M(T)$ of an AFM (see Fig. 1). The surface magnetization can be coupled to the magnetization of an adjacent ferromagnetic (FM) film, in a phenomenon called exchange bias (EB).^{1–3} Based on this, AFM/FM interfaces have been used to tune the properties of magnetic films and that together with the discovery of giant magneto-resistance⁴ brought on a technological revolution in spin engineering.^{5–7} Since then, research in antiferromagnets and AFM/FM interfaces has seen astonishing activity because of the new physics of interfacial magnetism^{8,9} and the technological importance of spin engineering.

The $M(T)$ of an AFM originates from uncompensated spins, and while it is intuitive that films with uncompensated surface planes would give interface exchange coupling, proportional to the surface magnetization of the AFM, the bias field^{10,11} has long been known to be only a few percent of the expected values.^{1–3} Experiments with exchange-coupled AFM films with uncompensated surfaces suggest that only a tiny percentage of the surface/interface spins participate in the coupling and even direct measurement of the net magnetization of uncompensated AFM resulted in a small percentage of the expected values.^{12,13} On the other hand, AFM with compensated surfaces, which should exhibit no coupling, reveal an EB that can be even

stronger than that of uncompensated surfaces,¹ which has been attributed to surface roughness and the formation of AFM domains.^{14–17}

This paper will show that, even in the absence of AFM domains, intrinsic effects exist that modify the expected magnetization of AFM films. Using Monte Carlo simulations, we will demonstrate that the surface and net magnetization of uncompensated AFM decrease non-monotonically with increasing roughness, that it does not scale with the surface area of thin films, and that it does not depend on the film thickness, i.e., it is also valid for bulk AFM systems. In addition, we will show that roughness generates non-collinear spin textures that further reduce the net magnetization of AFM. In this work, we did not consider AFM domains, since they are not the ground state.

In our simulations, we consider AFM films with uncompensated surfaces and induce roughness in the form of missing surface spins (and patches of spins) and steps. The latter form of roughness will have the strongest impact on the net magnetization, since monoatomic steps produce new compensation fronts in the modulated AFM structure and induce non-collinearity into the magnetization. Each step will introduce an additional uncompensated plateau with a magnetic moment that opposes that of the adjacent plateau (see Figs. 1(b) and 1(c), for example), resulting in a reduced net magnetization. We consider two cases: (i) constant thickness (Fig. 1(b)), such as would be found in a multilayer that develops roughness in a layer underlying the AFM, and (ii) varying thickness (Fig. 1(c)), such as would occur for a film grown on an atomically-flat substrate. The difference between the cases is that in (i) the surface magnetization is equal in both surfaces, whereas in (ii) the bottom surface is not affected by roughness.

^{a)}charilaou@mat.ethz.ch.

FIG. 1. Thin antiferromagnets in the Néel state with and without steps. Spins in the same atomic plane point in the same direction, indicated by the arrows, such that the magnetization of each plane is antiparallel to that of the adjacent planes. The top film (a) shows a perfect uncompensated flat antiferromagnet with 5 atomic planes. Panel (b) shows an uncompensated AFM with 5 atomic planes, and six conformal steps (7 plateaus), where the net magnetization is equal to $1/7$. Panel (c) shows an AFM with flat bottom atomic plane and rough top surface with thicker and thinner areas; here the net magnetization is equal to $4/7$. While these examples show systems where the change in thickness is monotonic, the results apply to non-monotonic varying thickness as well, i.e., when some steps go up and some steps go down. The length of each arrow in each atomic plane indicates how the magnetic moment at the surface is weaker at finite temperature.

II. MODEL AND COMPUTATION

The AFM films were made of hexagonally ordered ferromagnetic atomic planes stacked in an ABC repetition and antiferromagnetically coupled to each other, to simulate the structure of epitaxial (111) metal-oxide films like CoO, which have the NaCl structure. In this structure, each magnetic ion has 12 nearest neighbors: 6 within each (111) plane and 3 in each of the adjacent (111) planes. Below the Néel temperature T_N the cubic crystal symmetry breaks into a rhombohedral symmetry, such that not all the bonds with the 12 nearest neighbors are equivalent,¹⁸ resulting in a type G AFM ordering. For a detailed description of the structure, see, e.g., Ref. 19. The films had a thickness of $D = 15$ atomic planes, which corresponds to a thickness of 3.6 nm in real films, and a lateral size of $L \times L = 150 \times 150$ spins. Periodic boundary conditions were used in the two lateral dimensions to eliminate finite-size effects, whereas open boundaries were used for the top and bottom surfaces. Occasional checks were performed with larger systems ($L \times L = 200 \times 200$) to confirm that our results do not depend on the size of the simulated system.

Simulations were performed with the Heisenberg model, with the Hamiltonian

$$\mathcal{H} = -\frac{1}{2} \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j - K \sum_i (S_i^x)^2, \quad (1)$$

where J_{ij} is the exchange coupling between the spin vectors $\vec{S}_i$ and $\vec{S}_j$, which are normalized to $|\vec{S}| = 1$. The exchange

coupling is positive for intra-plane interactions ($J = 1$) and negative for inter-plane interactions ($J^* = -1$). The second term defines the anisotropy of the system, which was set along the x direction, i.e., to simulate the in-plane magnetization of CoO, which lies in the $[11\bar{1}]$ direction.²⁰ The anisotropy constant K was scaled to J as $K/J = 0.1$, i.e., an order of magnitude smaller than the exchange energy since K is on the order of 0.5–1 meV (Ref. 21) whereas J is on the order of 6–10 meV.²² Each spin interacts via J with its 6 nearest neighbors (nn) inside the same plane, and via J^* with the 3 nn in each of the adjacent planes. Based on the above Hamiltonian, spins which are in the same atomic plane will tend to order parallel to minimize the energy, and spins which are in adjacent planes will tend to align antiparallel. The Monte Carlo method is the best choice for finding the energy minimum, since it can be used to solve the Hamiltonian of any interacting many-body system.

The thermalization of the spin structure was performed via the Metropolis algorithm, i.e., by updating a single spin each time until the system comes to quasi-equilibrium. At each step of the thermalization, a single spin is chosen at random and its direction is changed. If the energy of the system becomes lower through that change, the change is accepted. If the energy becomes higher, the change is accepted by the Boltzmann probability $\exp(-\Delta\mathcal{H}/T)$, where $\Delta\mathcal{H}$ is the energy change caused by the spin flip, and T is the temperature of the system. This process was repeated for 2000 times per spin to find the equilibrium of the system, and then an additional 10^8 steps were taken to measure the thermodynamic average of the net magnetization of the system $M(T)$, which is the normalized sum of all spins (we normalized M so that $M = 1$ means that M is equal to the magnetization of a single atomic plane, e.g., that of the surface). The temperature was swept from $T = 0$ (fully ordered Néel state) to $T = 1.2 T_N$ (paramagnetic state), where T_N is the Néel temperature of the film, which for $D = 15$ is very close to the bulk value.²³

III. RESULTS AND DISCUSSION

A. Films with roughness in form of steps

Figure 2 shows the $M(T)$ curves of AFM with a thickness of $D = 15$, with increasing number of steps. For a perfectly flat film (1 plateau, 0 steps; see Fig. 1(a)), the $M(T)$ curve has a nearly linear shape, which is different from the Brillouin shape of $M(T)$ in FM materials due to finite size effects.^{23,24} Starting from $M = 1$ at $T = 0$, i.e., the net magnetization is equal to the magnetization of one atomic (111) plane and decreases monotonically with increasing T . At finite T , the net magnetization is not equal to the surface magnetization due to the profile through the thickness of the AFM: the two surfaces have equal m_s , with the same sign, and they are partially but not completely compensated by the two atomic planes beneath them, and in turn the next two planes partially offset that difference (see Fig. 1(a) where this is shown schematically in the length of the arrows). Because the surface spins have reduced coordination compared to spins inside the film, the surface magnetic moment has a different temperature dependence than the interior

FIG. 2. Net magnetization as a function of temperature for AFM with $D = 15$ atomic planes and increasing number of plateaus N . For a film with only one plateau, the magnetization at $T = 0$ is equal to 1 and corresponds to the magnetization of the uncompensated surface. For a film with 3 plateaus the magnetization becomes $1/3$, and for the film with 9 plateaus it becomes $1/9$. The inset shows how the decrease in M is described by a $1/N$ law, where M oscillates between 0 for even N and $1/N$ for odd N .

atomic planes of the film, and therefore the cancellation of magnetic moments in the AFM changes with temperature, resulting in the shown $M(T)$.

When we include roughness in the AFM, the steps introduce a FM domain structure to the net $M(T)$ of the AFM, as shown in Fig. 1, without the formation of any AFM domains. When there is an odd number of equidistant steps, i.e., an even number of plateaus, all of them cancel each other out and the net AFM M will be 0, but when the number of steps is even (number of plateaus is odd) $M \neq 0$. For example, when the AFM has two steps (three plateaus), the magnetization of two of the plateaus cancels out and only one of the three plateaus remains uncompensated, thus resulting in a saturation magnetization of $1/3$ at $T = 0$. As the number of steps is increased, the magnetization decreases by a factor of $1/N$ for odd N , and is zero when N is even, where N is the number of plateaus, thus exhibiting a distinct non-monotonic behavior as seen in the inset to Fig. 2.

We can describe the decrease of M by counting the number of plateaus (domains) N , assuming they have the same lateral size. At $T = 0$, where classically all the atomic planes have their saturation magnetization, then each plateau has a magnetization of $1/N$, and the total magnetization is the sum of the individual domain-states. Considering that each domain has a magnetization that opposes that of the adjacent domains, we can formulate the AFM magnetization simply as $M_{\text{AFM}} = (1/N) \sum_i (-1)^i$. Using this equation, we can extrapolate to a large number of steps, which would correspond to actual AFM films grown under laboratory conditions.

We find that the results of the Monte Carlo simulations are described perfectly by the $1/N$ trend (see inset to Fig. 2). The oscillatory behavior and the strong decay of the film magnetization with increasing number of steps are striking. If we extrapolate this trend for a large number of steps, corresponding to scales of μm , the magnetization of the AFM film is reduced to 1–5% of the total uncompensated spins,

which is the typical range found in experiments.^{12,13} This also explains the strongly reduced exchange bias field, which depends on the surface magnetization that is reduced by the occurrence of steps. Note, however, that this effect is not related to that described by Malozemoff,¹⁴ where with decreasing AFM domain size the bias field increases, as was observed in Ref. 25.

While our results are based on the occurrence of equidistant monoatomic steps, the validity of our finding remains intact for films with random plateau sizes. If we consider any distribution of plateau sizes the $1/N$ trend is still valid and the result is similar: the magnetization oscillates and decreases with increasing number of steps. The results are also unaltered when the steps in the film do not propagate in a specific direction, i.e., when some steps go up and some steps go down.

The situation changes when the steps occur for only one of the two surfaces (Fig. 1(c); results shown in Fig. 3). In this scenario, the bottom atomic plane is flat, while the top surface breaks into steps, and the thickness gradually changes over distance (as illustrated in Fig. 1(c)). In the example shown in Fig. 1(c), the AFM has a thickness of 11 atomic planes (uncompensated) at the left edge. After the monoatomic step, it has a thickness of 10 atomic planes (compensated), and so on. In contrast to the previous scenario, where each FM domain had a net moment opposing that of the adjacent domains, here all domains that have a non-zero magnetic moment point to the same direction, whereas all intervening domains have $M = 0$. Hence, at each step, the AFM changes between an uncompensated and a compensated state. The net magnetization shows an oscillatory behavior as a function of N , where M oscillates between $1/2$ and $(2 + N)/2N$ for odd N . This is valid not only when the thickness varies monotonically, but in any scenario where the film has thinner and thicker areas due to roughness of the top surface.

FIG. 3. Net magnetization as a function of temperature for AFM with varying thickness, depending on the number of plateaus N . For a film with only one plateau, the magnetization at $T = 0$ is equal to 1 and corresponds to the magnetization of the uncompensated surface. For a film with 2 plateaus the magnetization becomes $1/2$ and for the film with 9 plateaus it becomes $5/9$. The inset shows how the decrease in M is described by a $1/N$ law, where M oscillates between $1/2$ for even N and $(2 + N)/2N$ for odd N .

To better understand this behavior, we consider the following. For an AFM with two plateaus, there will be two domains: one with $M = 1/2$ and one with $M = 0$ (compensated). For an AFM with three plateaus, there will be two uncompensated and one compensated domain, and hence $M = 2/3$. In contrast to the previous scenario (with steps occurring at both surfaces), the net magnetization does not go to zero as the number of steps becomes large. Even in the limit of infinite number of steps, M will be finite and equal to $(2 + N)/2N = 1/2$ (see inset to Fig. 3). Note also that the magnetization of the AFM with roughness depends on the *local* thickness, because the magnetic moment at the surface is weaker than in the core of the film. Therefore, the magnetization profile becomes non-trivial and depends on the lateral dimension of the AFM (see Fig. 1(c) for a graphical explanation).

Because the cancellation of magnetic moments depends on the length scale of roughness, there is a striking lack of scaling of magnetization with surface area. For example, an AFM film with 7 plateaus, having a net magnetization of $1/7$, when split in two, e.g., a film with (i) 4 and another with (ii) 3 plateaus, will result in a net magnetization of 0 for film (i) and $1/3$ for film (ii) (relative to the surface area of the new film), and therefore the magnetization per surface area will increase. Further, if we split an AFM film with 6 plateaus, which has zero net magnetization, into two films with 3 plateaus each, both of them will exhibit a net magnetization per surface area of $1/3$ thus increasing the magnetization from zero to $1/3$. If we split the same film, however, in two films, one with 2 and one with 4 plateaus, the magnetization remains zero. Therefore, by changing the lateral size of a rough AFM film, the magnetization per surface area can change drastically.

B. Films with surface vacancies

Now we turn to films with roughness in the form of missing surface atoms. This can occur in real materials either in the form of surface vacancies or more commonly when patches of atoms are missing from the surface, corresponding to an incomplete atomic plane. We limit this study to surface vacancies only but note that vacancies deep inside the AFM can also have a drastic effect on the net magnetization. Here, we denote the surface roughness in terms of the atomic occupancy (O) of the surface. A value of 1.0 corresponds to a fully occupied surface, whereas 0.5 corresponds to a half-filled surface atomic plane, which is different than a single step because there is no edge in the structure.

We consider two situations: the case when only one surface is rough [Fig. 4(a)], and when both surfaces are rough [Fig. 4(b)]. As for roughness in the form of steps, the former can occur when an AFM film is deposited on a perfectly flat substrate, whereas the latter can occur in multilayers (with AFM and a spacer layer) due to mixing at each interface of the multilayer. Here, we will only discuss systems with an odd number of layers, specifically $D = 15$.

When only one surface is rough (shown in Fig. 4(a)), while the rest of the AFM is perfect, the net magnetization decreases linearly with decreasing occupancy. When

FIG. 4. Net magnetization of AFM with $D = 15$ with surface roughness, i.e., missing surface atoms. Panel (a) shows the results for films where only the top surface is rough, and panel (b) shows the results for films where both surfaces have the same amount of roughness. Four cases are shown for each situation: surface occupancy is 1.0 (squares), 0.75 (circles), 0.50 (triangles), and 0.25 (diamonds).

$O = 1.0$, corresponding to a perfect AFM, the saturation magnetization at $T = 0$ is equal to that of a single atomic plane. When the occupancy is reduced to 0.75, the saturation M is 0.75, and similarly, when $O = 0.5$ $M(T = 0) = 0.5$, and for $O = 0.25$ $M(T = 0) = 0.25$. The net saturation magnetization decreases linearly with decreasing surface occupancy, and in the limit of $O \rightarrow 0$, M will be zero because the AFM will then have an even number of atomic planes, where full compensation occurs.

The occupancy O changes not only the saturation value of M but also the shape of $M(T)$ (see Fig. 4(a)). This occurs because there are already fewer interactions among the surface spins even for no vacancies, the vacancies therefore create an even larger % effect on the reduced coordination of the surface spins, which in turn reduces the magnetic moment of the surface and affects its T -dependence therefore changing the degree of cancellation of magnetic moments beneath the surface. For $O = 1.0$, the $M(T)$ has the shape discussed previously, and as O is decreased, the curvature of $M(T)$ changes. Most notably, for $O = 0.25$ $M(T)$ exhibits a linear T -dependence.

If we consider the second case (see Fig. 4(b)), where both surfaces of the AFM have the same roughness, the effects of O on the saturation value and on $M(T)$ are more dramatic. When $O = 0.75$, the saturated net magnetization at $T = 0$ drops to 0.5, because the total magnetic moment of the surface planes amounts to $m_1 + m_{15} = 0.75 + 0.75 = 1.5$, and is compensated by the rest of the AFM, i.e., the other 13 atomic planes, which have a net moment of -1 . Note the drastic change in $M(T)$, which exhibits no transition at T_N (where the AFM ordering of the film occurs) but remains nearly zero for $0.8 \leq T/T_N \leq 1.0$ and then with decreasing temperature increases gradually towards $M = 0.5$. The change in the $M(T)$ is due to the alteration of the magnetization profile when both surfaces are rough, i.e., when they have a reduced m_s . At finite T the reduction of the surface

moments leads to a reduction of the second-to-surface moments, leading to a different T -dependence of the net M .

When we further decrease O on both surfaces, M has a *negative* onset at T_N (negative means that the direction of M opposes that of the spins on the surface). With decreasing temperature M increases in the negative direction, reaches a maximum around $T/T_N \approx 0.6$, and upon further decreasing T is reduced to $M=0$. With a surface occupancy of 0.5, at $T=0$ the net magnetic moment of the surfaces is fully compensated by the rest of the AFM. This is therefore the criterion for the occurrence of positive or negative M when both surfaces are rough. If $O > 0.5$, the magnetic moment of the surfaces will overcome that of the rest of the AFM and M will be positive, and when $O < 0.5$ the surface moments will be smaller than the rest, and M will be negative. Hence, when O is further decreased to 0.25, the net magnetization is negative at all T and saturates at $M = -0.5$.

Non-monotonic $M(T)$ can occur even for AFM with perfect surfaces when the exchange interaction between surface spins is modified compared to that of the bulk,²⁷ but roughness has a more dramatic impact on the $M(T)$ as seen here.

In comparing the two roughness mechanisms, i.e., steps vs. vacancies, the main difference is that steps change the thickness of the AFM. A monoatomic step changes the state of the AFM from uncompensated to compensated or vice versa, whereas surface vacancies only dilute the spin structure on the surface, without changing the thickness. In both cases, however, the dimensionality of the AFM will remain unchanged, despite the fact that a step is a 1D defect, whereas a single vacancy is a 0D defect.

The above results consider AFM with uncompensated surfaces. In the reverse scenario, i.e., a compensated AFM with an even number of atomic planes, roughness and defects would increase the concentration of uncompensated spins. At each step, a new front of uncompensated spins appears at the edge, and with additional steps, the total net magnetization increases with increasing number of steps (data not shown). In the case of AFM with compensated surfaces, such as FeMn(100), the net magnetization, and exchange bias field, increases with increasing roughness, as experimentally found by Kuch *et al.*²⁸ He *et al.*²⁹ used this in a stepped Cr_2O_3 single crystal to make use of the ferromagnetic alignment of the (0001) surface. Hence, the effect of roughness is reversed at compensated surfaces, where roughness (in the form of steps or patches) promotes ferromagnetism in AFM films.

C. Effects of roughness on the spin texture

We now turn our attention to the effects of roughness on the spin texture of the surfaces in AFM. The distribution of the net magnetization into plateaus corresponds to a formation of FM domains with antiparallel configuration. In this configuration, without including long-range dipolar interactions, the AFM is in the ground state, because all spin-spin bonds are satisfied. If, however, we include dipolar interactions in our calculation, we find that at each step edge, the surface spins are strongly affected by the step, even in the absence of anisotropy induced by changes in crystal fields at

step edges. This effect is similar to the dipolar-coupling induced perpendicular magnetic anisotropy deduced first by Néel for thin AFM films.^{30,31} To investigate this, we simulated AFM including long-range dipolar interactions using smaller sizes ($L \times L = 16 \times 16$ and $D=2$ due to the additional computational effort needed for this calculation). The long-range dipolar interactions are described by

$$\mathcal{H}_{\text{Dip}} = D \sum_{i \neq j} \left[\frac{\vec{S}_i \cdot \vec{S}_j}{r_{ij}^3} - 3 \frac{(\vec{S}_i \cdot \vec{r}_{ij})(\vec{S}_j \cdot \vec{r}_{ij})}{r_{ij}^5} \right], \quad (2)$$

where $D = S^2/4\pi$ is the dipolar coupling energy constant, and $\vec{r}$ is the vector connecting each two spin sites. For Co with a moment of $4\mu_B$, and $T_N = 300$ K (which corresponds to $J = 0.5$ meV per bond), D/J is 10^{-5} .

Since the size of the simulation system is limited (due to the increased computational effort), we employ a scaling law^{32,33} that allows us to simulate a larger system by scaling the energy ratio D/J . This means, in turn, that a single spin in the simulation corresponds to a group of spins in a real system. With increasing D/J ratio, the simulation system corresponds to an increasingly larger system.

Considering a plateau size of 100 nm, corresponding to roughly 320 atomic sites, the ratio between simulation size and real size is $16/320 = 0.05$. Given this, re-scaling the energies leads to $J_{\text{eff}} = 0.004J$ and consequently $D/J_{\text{eff}} = 0.0025$. For details about the scaling law, see Refs. 32 and 33.

Figure 5 shows the spin-texture of the atomic planes in an AFM bilayer with (a) a step edge, and (b) with a missing patch of surface atoms. In both cases, the spins on the physical edge of the system tend to align along the edge to minimize the dipolar interactions.³⁴ In the case of a sharp step, the step edge acts in a similar way and the spins align themselves parallel to the edge, deviating by 90° from their easy axis, in all atomic planes of the AFM structure. In the case of the missing patch of atoms (simulated by a circle), the spins on the surface tend to align themselves along the circumference of the circle, whereas the spins in the bottom atomic plane are not strongly influenced by the missing surface spins at $T \rightarrow 0$. In both cases, the collinearity of the AFM is lost, and the net magnetization will be reduced at $T=0$ and further reduced at finite T . Considering that spins on the surface are more strongly influenced by dipolar fields than spins inside the AFM, due to the broken symmetry, the magnetization profile is also affected in the sense that the surface magnetic moment is even weaker.

The geometry of the step edge is therefore critical for the spin structure. In the example shown in Fig. 5(a), the step edge is perpendicular to the easy axis of the anisotropy. In a scenario where the edge is parallel to the easy axis, there will be no change in the spin orientation close to the edge and the effect of roughness on the spin texture will be minimal.

Considering the dimensions of the system, long-range dipolar interactions will have a stronger impact with increasing physical size, i.e., with increasing plateau size. This means that spin-textures will play an important role when

FIG. 5. Spin texture of an AFM bilayer with roughness in form of (a) a step and (b) patch of missing surface atoms. In (a) the top image (red spins) shows the surface, which is discontinuous due to the step, the middle image (blue spins) shows the middle atomic plane, which is continuous, and the bottom image (red spins) shows the bottom surface. In (b) the top image shows the top surface spins (red) and the bottom image shows the bottom surface spins (blue). In both cases, the spins tend to align parallel to the edges.

plateaus are larger than $100\text{ nm} - 1\text{ }\mu\text{m}$, and that they will be negligible when the size of the plateaus will be smaller than $1 - 10\text{ nm}$. Given this, we can ascertain that roughness in the form of missing single spins, i.e., surface vacancies, will have the weakest impact on the spin texture, whereas roughness in the form of mesoscopic plateaus will have the strongest impact. Further, the geometry of the plateaus can generate a competition between exchange interaction and dipolar interactions due to the fact that the dipolar fields between plateaus may promote either ferromagnetic or antiferromagnetic coupling depending on the size and position of the plateaus, as shown analytically in Ref. 26 for interacting layers.

IV. ROLE OF ROUGHNESS IN DEVICE TECHNOLOGY

Considering the above findings, we now discuss the implications of roughness in AFM on the performance of devices, such as exchange-biased systems¹⁻³ and AFM-based magnetic semiconductors¹³ and offer suggestions for improvements including the possibility of taking advantage of a roughness-induced compensation point. The reduced net and surface magnetization resulting from roughness, either in the form of steps or surface vacancies, will strongly affect the coupling at interfaces between AFM and FM and result in a strongly reduced bias field. Similarly, in AFM-based magnetic semiconductors, the reduced net magnetization will lead to a strongly reduced net magnetic moment of the heterostructure, as evidenced in Ref. 13. Flat surfaces and

interfaces will increase the performance of AFM/FM heterostructures for uncompensated orientations but increased roughness will be helpful for compensated orientations, allowing for domains to form. Roughness even provides the possibility for designing novel heterostructures with highly tunable temperature-dependence of the net magnetic moment, offering possibilities for improved design of thermally assisted exchange bias systems. In the case of surface vacancies on both surfaces of the AFM, relatively straightforward to accomplish in a multilayer structure or by deliberately introducing adatoms both before and after the AFM deposition, one can create a compensation point by controlling the surface occupancy. This will enable the design of temperature-sensitive switches or the development of other sensor technologies.

One has to consider the fact that the spin texture at the interface between AFM and FM is altered by the exchange interaction³⁵ but even then the uncompensated AFM spins are pinned and not affected by external fields.³⁶ Moreover, extrinsic parameters may influence the spin texture at the interface, such as, e.g., intermixing between AFM and FM, such as in NiO/NiFe multilayers.³⁷ Such an intermixing can dramatically decrease the performance of the exchange coupling, but it can also enhance the magnetization at the interface, as seen in experiments³⁸ and *ab-initio* calculations³⁹ for the CoO/NiFe system.

Further, the modification of the spin texture on rough surfaces allows the design of novel structures, where steps or holes can produce different effects at different parts of the same film by patterning the structure of the substrate before deposition, or perhaps the film itself. The exchange bias will be locally modified in the patterned regions and new phenomena could be observed in the spin texture of the film, e.g., artificial spin ice structures.

V. CONCLUSIONS

We conclude that roughness in thin AFM films can modify the $M(T)$ completely and result in a nearly zero, or even negative M . In films with sharp steps the magnetization decreases non-monotonically with increasing number of steps. When roughness is limited to the surface atomic planes, in the form of vacancies, the magnetization decreases monotonically with increasing roughness, and a compensation point in $M(T)$ occurs due to the change in the magnetization profile. Moreover, the roughness can change the orientation of the magnetic moments and will tend to align spins along the step edges to lower the energy. These findings provide an explanation for several experimental observations that found only a small fraction of the anticipated net magnetization in uncompensated AFM films and also of the typically strongly reduced exchange bias field found in AFM/FM heterostructures and show that roughness in AFM can be used to design novel devices, where the local spin texture near steps or holes will lead to modified exchange bias.

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