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In-plane magnetic reorientation in coupled ferro- and antiferromagnetic thin films

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By studying coupled ferro- (FM) and antiferromagnetic thin-film systems, we obtain an in-plane magnetic reorientation as a function of temperature and FM film thickness. The interlayer exchange coupling causes a uniaxial anisotropy, which may compete with the intrinsic anisotropy of the FM film. Depending on the latter the total in-plane anisotropy of the FM film is either enhanced or reduced. Eventually a change of sign occurs, resulting in an in-plane magnetic reorientation between a collinear and an orthogonal magnetic arrangement of the two subsystems. A canted magnetic arrangement may occur, mediating between these two extremes. By measuring the anisotropy below and above the Néel temperature the interlayer exchange coupling can be determined. The calculations have been performed with a Heisenberg-like Hamiltonian by application of a two-spin mean-field theory.

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The interface between coupled ferro- (FM) and antiferromagnetic (AFM) films or particles has been attracted much interest recently, in particular due to the renewed interest in exchange biased systems for application in magnetoresistive sensors.[1,2] Of particular interest is the case of a ''compensated'' AFM interface with an equal number of positive and negative exchange interactions across the interface. By considering only exchange couplings, it has been shown by Koon that the most stable magnetic arrangement for such an interface is an orthogonal magnetic orientation of the FM and AFM subsystems.[3] A nonvanishing magnetic binding energy is obtained if the magnetic moments of the AFM are allowed to deviate from their equilibrium AFM arrangement, exhibiting thus a noncollinear AFM magnetization with a small component parallel or antiparallel to the FM, the ''spin-flop-phase.''[4] From the viewpoint of the FM film, the net magnetic binding energy introduces an in-plane uniaxial magnetic anisotropy $K_{\rm int}$.[5] A simple estimate[6] yields the strength of this interface anisotropy to be of the order $K_{\rm int} \propto -(J_{\rm int})^2/|J_{\rm AFM}|$, with $J_{\rm int}$ the interlayer exchange coupling between neighboring FM and AFM spins across the interface, and $J_{\rm AFM}$ the exchange coupling in the AFM system. Experimentally, collinear as well as orthogonal magnetic arrangements of coupled FM-AFM systems have been observed.[1,7]

Evidently, the magnetic direction of the FM film depends also on its intrinsic anisotropy $K_{\rm FM}$. If $K_{\rm int}$ and $K_{\rm FM}$ favors the same in-plane easy axis, the total anisotropy is enhanced.[8] If the two anisotropic contributions favors different magnetic directions, an in-plane magnetic reorientation may occur as a function of the FM film thickness, since $K_{\rm int}$ is proportional to the interface area, whereas $K_{\rm FM}$ is porportional to the volume of the FM film.

Quite interestingly, also a different temperature behavior of these two competing anisotropies may result in an in-plane magnetic reorientation. At finite temperatures T the magnetic direction is determined by effective, temperature-dependent anisotropies $\mathcal{K}(T)$, which depend on T mainly through the relative magnetization $M(T)$ as can be shown by a perturbative treatment.[9,10] In the present case of a coupled FM-AFM system the main reason for the different behavior of $\mathcal{K}_{\rm FM}(T)$ and $\mathcal{K}_{\rm int}(T)$ is the different ordering temperature of the two subsystems. If the Curie temperature T_C of the FM film is larger than the Néel temperature T_N of the AFM system, then for $T>T_N$ the magnetic direction of the FM film is exclusively determined by $\mathcal{K}_{\rm FM}(T)$, whereas below T_N it depends on the relative strength of $\mathcal{K}_{\rm FM}(T)$ and $\mathcal{K}_{\rm int}(T)$. Hence, the total anisotropy of the FM film $\mathcal{K}_{\rm tot,FM}(T)=\mathcal{K}_{\rm FM}(T)+\mathcal{K}_{\rm int}(T)$ possibly exhibits a change of sign as a function of temperature, and an in-plane magnetic reorientation occurs.

To our knowledge, such a magnetic reorientation in coupled FM-AFM thin-film systems has not been reported yet. In the present study we will investigate this phenomenon by determining the magnetic arrangement and the temperature-dependent anisotropies $\mathcal{K}_{\rm FM}(T)$ and $\mathcal{K}_{\rm int}(T)$. A Heisenberg-like Hamilton operator is applied with localized quantum spins $\mathbf{S}_i$ and spin quantum number $S=1$ on a simple cubic (001) lattice:

$$\mathcal{H}=-\frac{1}{2}\sum_{\langle i,j\rangle} J_{ij}\mathbf{S}_i\mathbf{S}_j-\sum_i K_i(S_i^z)^2. \qquad (1)$$

The FM and AFM films are assumed to consist of $n_{\rm FM}$ and $n_{\rm AFM}$ atomic layers, spanned by the xz plane. A compensated AFM interface is considered, which is accounted for by using two sublattices per layer.[11] The exchange interaction J_{ij} couples nearest-neighbor spins on lattice sites i and j. Caused by the shape anisotropy resulting from the dipole interaction, the magnetizations $\mathbf{M}_i=\langle\mathbf{S}_i\rangle$ are confined to the film plane. Furthermore, we assume a layer-dependent second-order in-plane uniaxial anisotropy K_i, favoring for $K_i>0$ an easy axis along the z direction and for $K_i<0$ along the x direction.[12] The FM and AFM subsystems are characterized by the exchange couplings $J_{\rm FM}$ and $J_{\rm AFM}$, and by the intrinsic anisotropies $K_{\rm FM}$ and $K_{\rm AFM}$. For these quantities typical values are taken into account. An anisotropy for the AFM is required, since otherwise it will start to rotate in accordance with the FM film. We do not distinguish here between surface or interface anisotropies different from those of the film interior layers, although they might differ considerably.[13]

The FM and AFM films are coupled across the interface by the interlayer exchange coupling $J_{\rm int}$.

The site-dependent in-plane magnetizations $\mathbf{M}_i(T)$ and free energies $F_i(T)$ are calculated within a mean-field theory. To take into account at least partly the strong correlations in the AFM, we apply here a two-spin-cluster (Oguchi-) method,[14] with both spins located in the same layer. Within this method the interactions in the cluster are treated exactly, whereas the remaining system is considered by a molecular field. The free energies and expectation values are determined by diagonalizing the corresponding two-spin matrices. We emphasize that the effective anisotropies are neither approximated by the low-temperature estimate[9] $\mathcal{K}(T) \sim M^{l(l+1)}(T)$, l the order of the anisotropy, nor by a thermodynamic perturbation theory.[10] This allows for an appropriate treatment of the anisotropies also near and above ordering temperatures.

Caused by $J_{\rm int}$ the spins of the AFM layers especially close to the interface may deviate from their undisturbed equilibrium directions. For simplicity, due to the strong FM exchange interaction a collinear magnetization of the whole FM film is assumed, which will be rotated by the in-plane angle $\phi_{\rm FM}$. The magnetizations $|\mathbf{M}_{\rm i,FM}|(T)$ of the FM layers, and the two magnetization components $M^x_{\rm i,AFM}(T)$ and $M^z_{\rm i,AFM}(T)$ of the AFM layers are determined by minimizing the total free energy $F(T,\phi_{\rm FM})=\Sigma_i F_i(T,\phi_{\rm FM})$ with the help of a conjugated gradient method. The minimum of $F(T,\phi_{\rm FM})$ yields the equilibrium angle $\phi_{0,\rm FM}$ of the FM film magnetization. The total anisotropy $\mathcal{K}_{\rm tot,FM}(T)$ per FM spin is calculated from the free energy difference between the orthogonal ($\phi_{\rm FM}=\pi/2$) and the collinear ($\phi_{\rm FM}=0$) magnetic arrangement:

$$\mathcal{K}_{\rm tot,FM}(T)=\frac{1}{n_{\rm FM}}[F(T,\phi_{\rm FM}=\pi/2)-F(T,\phi_{\rm FM}=0)]. \tag{2}$$

The following results are calculated assuming representative values for the exchange and anisotropy parameters in units of $J_{\rm FM}$. If not stated otherwise, we use $J_{\rm AFM}/J_{\rm FM}=-0.5$ and $|K_{\rm FM}/J_{\rm FM}|=K_{\rm AFM}/J_{\rm FM}=0.01$. For the thicknesses of the FM and AFM films we assume $n_{\rm FM}=5$ and $n_{\rm AFM}=10$. From these values the critical temperatures $T_C/J_{\rm FM}=3.68$ and $T_N/J_{\rm FM}=1.92$ are obtained for $J_{\rm int}=0$.

In Fig. 1 we show the total effective anisotropy per FM spin as a function of temperature T, where we depict different scenarios. A positive value of $\mathcal{K}_{\rm tot,FM}(T)$ favors a magnetic direction of the FM film along the z-axis collinear to the AFM magnetization (collinear arrangement), and a negative value a direction along the x axis (orthogonal arrangement). The solid line (a) refers to the intrinsic anisotropy $\mathcal{K}_{\rm FM}(T)$ of the FM film for the uncoupled case ($J_{\rm int}=0$). The $\mathcal{K}_{\rm FM}(T)$ decreases with increasing temperature and vanishes for $T>T_C$, as has been calculated and measured for many different FM thin-film systems.[13] This does not imply that the underlying spin-orbit coupling varies with temperature. Rather due to the increasing thermal agitation the ability of the anisotropy to maintain a particular direction of the magnetization decreases. The dashed line (b) shows the interface

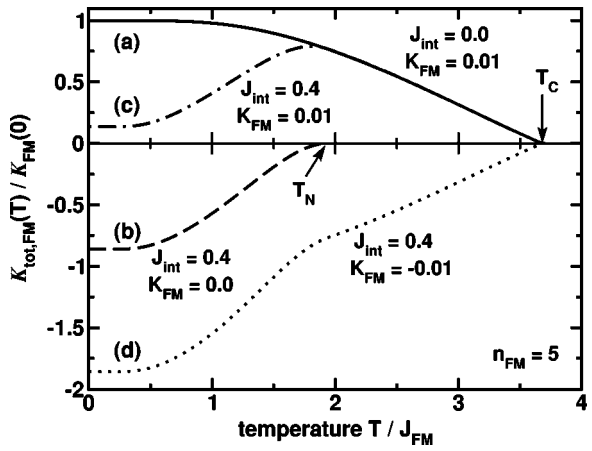

FIG. 1. Total effective anisotropy $\mathcal{K}_{\rm tot,FM}(T)$ per spin of the FM film as a function of temperature T. The $\mathcal{K}_{\rm tot,FM}(T)>0$ prefers a collinear, and $\mathcal{K}_{\rm tot,FM}(T)<0$ an orthogonal FM film magnetization with respect to the AFM magnetic direction. The exchange couplings, intrinsic anisotropies, and temperatures are given in units of $J_{\rm FM}$, and $\mathcal{K}_{\rm tot,FM}(T)$ in units of $K_{\rm FM}=\mathcal{K}_{\rm FM}(T=0)$. We assume $J_{\rm AFM}/J_{\rm FM}=-0.5$ and $K_{\rm AFM}/J_{\rm FM}=0.01$, in addition $n_{\rm FM}=5$ and $n_{\rm AFM}=10$ for the thicknesses of the FM and AFM films. For these values the Curie temperature T_C of the FM film is greater than the Néel temperature T_N of the AFM film. The full line (a) shows the intrinsic anisotropy for a decoupled FM film ($J_{\rm int}=0$) for $K_{\rm FM}/J_{\rm FM}=0.01$. The dashed line (b) refers to the bare interface anisotropy ($K_{\rm FM}=0$), assuming $J_{\rm int}/J_{\rm FM}=0.4$. The presence of both anisotropic contributions results in a reduced $\mathcal{K}_{\rm tot,FM}(T)$, dot-dashed line (c). For $K_{\rm FM}/J_{\rm FM}=-0.01$ an enhanced absolute value $|\mathcal{K}_{\rm tot,FM}(T)|$ is obtained, dotted line (d).

anisotropy $\mathcal{K}_{\rm int}(T)$ for a vanishing intrinsic FM anisotropy, assuming $J_{\rm int}/J_{\rm FM}=0.4$. Evidently, $\mathcal{K}_{\rm int}(T)$ assumes a finite value for an ordered AFM phase, and disappears above the Néel temperature T_N. If both anisotropic contributions are present, the resulting total effective anisotropy $\mathcal{K}_{\rm tot,FM}(T)$ is approximately given by the sum of $\mathcal{K}_{\rm int}(T)$ and $\mathcal{K}_{\rm FM}(T)$, see the dot-dashed line (c). Finally, by assuming $K_{\rm FM}/J_{\rm FM}=-0.01$ the dotted line (d) refers to the case of an intrinsic FM anisotropy favoring the same easy axis than $K_{\rm int}$. Therefore, the absolute value $|\mathcal{K}_{\rm tot,FM}(T)|$ may be either reduced (c) or enhanced (d) by the interlayer exchange coupling. We emphasize that for the former case the two anisotropies $\mathcal{K}_{\rm FM}(T)$ and $\mathcal{K}_{\rm int}(T)$ compete, resulting possibly in a change of sign of $\mathcal{K}_{\rm tot,FM}(T)$, and thus in an in-plane magnetic reorientation of the FM film with varying temperature.

Such a magnetic reorientation can be observed in Fig. 2, where we present $\mathcal{K}_{\rm tot,FM}(T)$ for different values of the interlayer exchange coupling $J_{\rm int}$ and for the FM film thickness $n_{\rm FM}=5$. Furthermore, Fig. 3 shows $\mathcal{K}_{\rm tot,FM}(T)$ for different $n_{\rm FM}$, assuming $J_{\rm int}/J_{\rm FM}=0.4$. The chosen parameters yield $T_C>T_N$. As mentioned, $K_{\rm FM}$ favors an easy axis collinear to the AFM magnetization. $\mathcal{K}_{\rm tot,FM}(T)$ changes sign at the reorientation temperature T_R for a strong $J_{\rm int}$ or for a small $n_{\rm FM}$. For $T>T_R$ a collinear, and for $T<T_R$ preferably an orthogonal magnetic arrangement results. This can be seen from the continuously varying equilibrium FM angles $\phi_{0,\rm FM}$, which are also depicted in Figs. 2 and 3. We emphasize that the

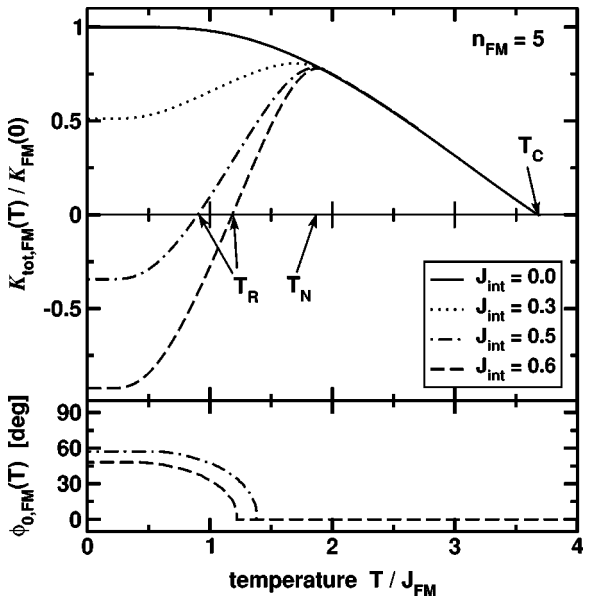

FIG. 2. Total effective anisotropy $\mathcal{K}_{\mathrm{tot,FM}}(T)$ per FM film spin as a function of temperature for different interlayer exchange couplings J_{int}, assuming $n_{\mathrm{FM}}=5$. The reorientation temperature T_R is defined by the change of sign of $\mathcal{K}_{\mathrm{tot,FM}}(T)$. In addition the equilibrium angles $\phi_{0,\mathrm{FM}}(T)$ of the FM film magnetization for $J_{\mathrm{int}}/J_{\mathrm{FM}}=0.5$ and $J_{\mathrm{int}}/J_{\mathrm{FM}}=0.6$ are displayed, indicating a continuous magnetic reorientation near T_R.

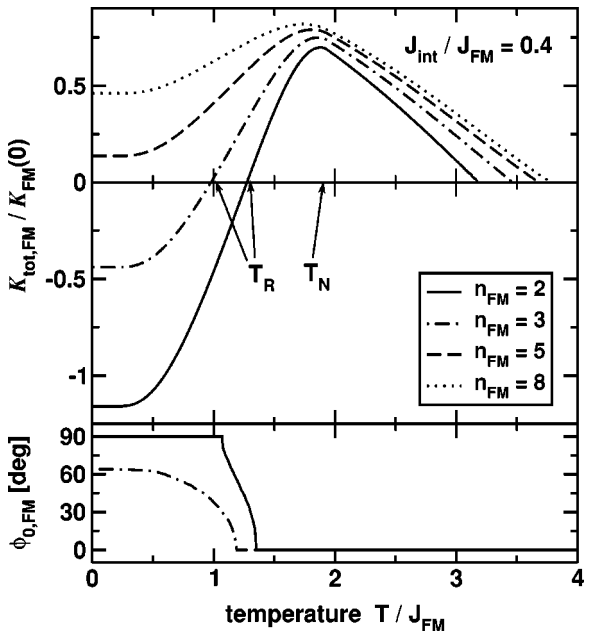

FIG. 3. Total effective anisotropy $\mathcal{K}_{\mathrm{tot,FM}}(T)$ per FM film spin as a function of temperature for different FM film thicknesses n_{FM}, assuming $J_{\mathrm{int}}/J_{\mathrm{FM}}=0.4$. The equilibrium angles $\phi_{0,\mathrm{FM}}(T)$ of the FM film magnetization are shown for $n_{\mathrm{FM}}=2$ and $n_{\mathrm{FM}}=3$. The reorientation temperature is denoted by T_R. Whereas for $n_{\mathrm{FM}}=2$ a reorientation between the collinear and orthogonal magnetic arrangements is obtained, for $n_{\mathrm{FM}}=3$ a canted arrangement is present at low temperatures.

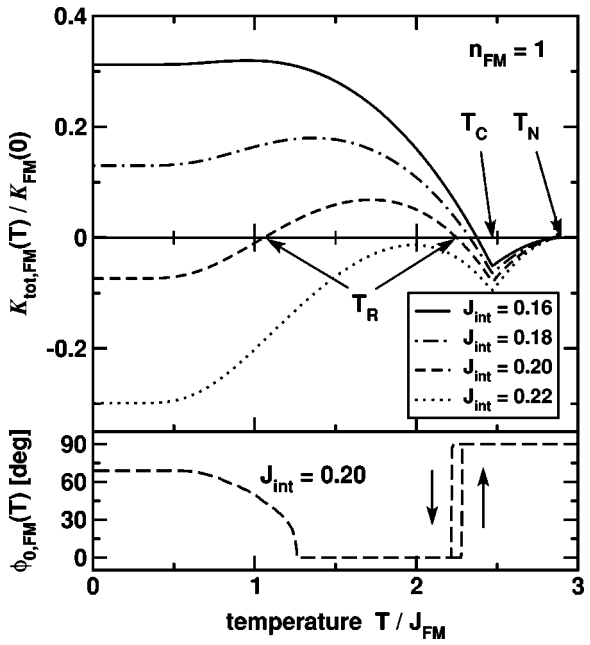

FIG. 4. Total effective anisotropy $\mathcal{K}_{\mathrm{tot,FM}}(T)$ per FM film spin as a function of temperature for different interlayer exchange couplings J_{int}, assuming $n_{\mathrm{FM}}=1$ and $J_{\mathrm{AFM}}/J_{\mathrm{FM}}=-0.75$. For these values one obtains $T_C<T_N$. The equilibrium angle $\phi_{0,\mathrm{FM}}(T)$ of the FM film magnetization is shown for $J_{\mathrm{int}}/J_{\mathrm{FM}}=0.2$. For this value a reentrant magnetic behavior is obtained, indicated by changes of sign of $\mathcal{K}_{\mathrm{tot,FM}}(T)$ near the reorientation temperatures T_R, and a hysteresis close to T_C.

orthogonal arrangement ($\phi_{0,\mathrm{FM}}=\pi/2$) is not always realized. Rather, dependent on the interaction parameters, a canted magnetic arrangement between the FM and the AFM subsystems may occur, characterized by an equilibrium angle $0<\phi_{0,\mathrm{FM}}<\pi/2$. In this case the free energy $F(T,\phi_{\mathrm{FM}})$ as a function of ϕ_{FM} exhibits four minima rather than two as for a simple uniaxial anisotropy.[15] A twofold symmetry is still present. For very strong J_{int} also hysteresis effects may occur by varying ϕ_{FM}, accompanied by sudden jumps of the AFM spin angles ϕ_i (spin-flop-transition).[4,5,16] The AFM film exhibits a noncollinear, spin-flop-like magnetic arrangement for $\phi_{0,\mathrm{FM}}>0$. Furthermore, an in-plane magnetic reorientation with an increasing FM film thickness n_{FM} for a constant temperature can be observed in Fig. 3. A small value for $|\mathcal{K}_{\mathrm{tot,FM}}(T)|$ may occur, corresponding to a very soft ferromagnet. We note that $\mathcal{K}_{\mathrm{tot,FM}}(T)$ does not depend on the sign of J_{int}, consistent with the estimate[6] $K_{\mathrm{int}}\propto-(J_{\mathrm{int}})^2/|J_{\mathrm{AFM}}|$. The disturbance of the AFM spins in the spin-flop-phase decreases rapidly with increasing distance from the interface.[8]

In addition, we present results for the case for which the Curie temperature T_C is smaller than the Néel temperature T_N. The correspondent $\mathcal{K}_{\mathrm{tot,FM}}(T)$ is shown in Fig. 4 for different interlayer exchange couplings J_{int}. By assuming $n_{\mathrm{FM}}=1$ and $J_{\mathrm{AFM}}/J_{\mathrm{FM}}=-0.75$, we obtain $T_C/J_{\mathrm{FM}}=2.47$ and $T_N/J_{\mathrm{FM}}=2.90$. An in-plane magnetic reorientation of the FM film close to T_C is obtained, if J_{int} is not too strong. However, the order of the respective magnetic arrangements is reversed with respect to the case $T_C>T_N$. In the range $T_C<T<T_N$ a small magnetic order and a small interface

anisotropy $\mathcal{K}_{\rm int}(T)$ is induced in the FM film, resulting in an orthogonal magnetic arrangement. For $T<T_C$ the intrinsic FM anisotropy $\mathcal{K}_{\rm FM}(T)$ becomes increasingly important and may cause a magnetic reorientation into the collinear arrangement with a decreasing temperature. Furthermore, an intermediate value of $J_{\rm int}$ can result in a reentrant magnetic behavior, i.e., at lower temperatures a second reorientation into a canted magnetic arrangement takes place. This behavior can be observed from the equilibrium angle $\phi_{0,\rm FM}$, which is also shown in Fig. 4 for $J_{\rm int}/J_{\rm FM}=0.2$. A continuous variation of $\phi_{0,\rm FM}$ is obtained for low temperatures, and a discontinuous one close to T_C, accompanied by a hysteretic behavior. Note that the results are obtained under the assumption that the magnetization of the FM film stays always parallel. This assumption is questionable for temperatures $T_C<T<T_N$.

The strength of $J_{\rm int}$ is not well known. It depends on the material combination, the morphology, and the presence of impurities near the interface. It has been proposed to measure $J_{\rm int}$ by applying an external magnetic field, inducing a spin-flop transition in the AFM subsystem.[16] However, to create such a spin-flop transition the magnetic field must possibly be very strong. We propose that $J_{\rm int}$ can be determined by measuring the total anisotropy $\mathcal{K}_{\rm tot,FM}(T)$ of the FM film above and below T_N, requiring $T_N<T_C$.

In coupled FM-AFM systems also the exchange bias or the unidirectional anisotropy is observed,[1,2] which is characterized by an asymmetric hysteresis loop. Whereas the origin of this important quantity is still not completely resolved, the occurrence of the exchange bias is most likely caused by a certain amount of interface roughness, defects, and noncompensated AFM spins,[5,17] accompanied possibly by a domain phase in the AFM subsystem.[18] In the actual study this phenomenon has not been adressed.

To conclude, we point out the possibility of an in-plane magnetic reorientation in coupled FM-AFM thin films. By application of a mean-field theory we have calculated the effective magnetic anisotropy, the magnetic arrangement, and the equilibrium direction of the FM film for such systems. The interlayer exchange coupling $J_{\rm int}$ causes an interface anisotropy $\mathcal{K}_{\rm int}(T)$, which adds to the intrinsic anisotropy $\mathcal{K}_{\rm FM}(T)$ of the FM film, and vanishes above the Néel temperature T_N of the AFM system. Depending on the sign of $\mathcal{K}_{\rm FM}(T)$, the total anisotropy $\mathcal{K}_{\rm tot,FM}(T)$ of the FM film may be enhanced as well as be reduced, see Fig. 1. For competing intrinsic and interlayer anisotropies a magnetic reorientation of the FM film magnetization may occur with increasing temperature T or a varying FM film thickness $n_{\rm FM}$, as shown in Figs. 2–4. The main reason for the temperature induced in-plane reorientation is the different ordering temperature of the two subsystems, causing a different temperature dependency of $\mathcal{K}_{\rm FM}(T)$ and $\mathcal{K}_{\rm int}(T)$. The magnetizations of the FM and AFM films can be either collinear or orthogonal to each other. In addition a canted magnetic arrangement may occur. Hence, the assumption that the magnetic structures in coupled FM-AFM systems are either collinear[18] or orthogonal[2,3] is not always true. The noncollinear, spin-flop-like arrangement of the AFM spins[4,5] for $\phi_{0,\rm FM}>0$ vanishes rapidly with increasing distance from the FM-AFM interface.

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