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

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By studying coupled ferro- (FM) and antiferromagnetic (AFM) 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. 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 N.C. Koon that the most stable magnetic arrangement for such an interface is an orthogonal magnetic orientation of the FM and AFM subsystems. 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 magnetic reorientation. At finite temperatures the magnetic direction is determined by effective, temperature dependent anisotropies $K_{\text{int}}$. Hence, the total anisotropy of the FM film $K_{\text{tot,FM}} = K_{\text{FM}}(T) + K_{\text{int}}(T)$ 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 $K_{\text{FM}}(T)$ and $K_{\text{int}}(T)$. A Heisenberg-like Hamilton operator is applied with localized quantum spins $S_i$ and spin quantum number $S=1$ on a simple cubic (001) lattice:

$$H = -\frac{1}{2} \sum_{(i,j)} J_{ij} S_i S_j - \sum_i K_i (S_i^z)^2.$$  

(1)

The FM and AFM films are assumed to consist of $n_{\text{FM}}$ and $n_{\text{AFM}}$ atomic layers, spanned by the $xz$-plane. A compensated AFM interface is considered, which is accounted for by using two sublattices per layer. 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 $M_i = \langle S_i \rangle$ 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 $z$- and for $K_i < 0$ along the $x$-direction. The FM and AFM subsystems are characterized by the exchange couplings $J_{\text{FM}}$ and $J_{\text{AFM}}$, and by the intrinsic anisotropies $K_{\text{FM}}$ and $K_{\text{AFM}}$. 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. FM and AFM are coupled across the interface by the interlayer exchange coupling $J_{\text{int}}$.

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 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 $K(T) \sim M_i^{(l+1)}(T)$, $l$ the order of the anisotropy, nor by a thermodynamic perturbation theory. This allows for an appropriate treatment of the anisotropies also near and above ordering temperatures.

Caused by $J_{\text{int}}$ 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 $\phi_{\text{FM}}$. The magnetizations $|\mathbf{M}_{\text{FM}}(T)|$ of the FM layers, and the two magnetization components $M_{\phi,\text{AFM}}(T)$ and $M_{\chi,\text{AFM}}(T)$ of the AFM layers are determined by minimizing the total free energy $F(T, \phi_{\text{FM}}) = \sum_i F_i(T, \phi_{\text{FM}})$ with the help of a conjugated gradient method. The minimum of $F(T, \phi_{\text{FM}})$ yields the equilibrium angle $\phi_{\text{FM}}$ of the FM film magnetization. The total anisotropy $K_{\text{tot},\text{FM}}(T)$ per FM spin is calculated from the free energy difference between the orthogonal ($\phi_{\text{FM}} = \pi/2$) and the collinear ($\phi_{\text{FM}} = 0$) magnetic arrangement:

$$K_{\text{tot},\text{FM}}(T) = \frac{1}{n_{\text{FM}}} \left[ F(T, \phi_{\text{FM}} = \pi/2) - F(T, \phi_{\text{FM}} = 0) \right]. \tag{2}$$

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

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 $K_{\text{tot,FM}}(T)$ 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 $K_{\text{FM}}(T)$ of the FM film for the uncoupled case ($J_{\text{int}} = 0$). $K_{\text{FM}}(T)$ decreases with increasing temperature and vanishes for $T > T_C$, as has been calculated and measured for many different FM thin film systems. 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 anisotropy $K_{\text{tot}}(T)$ for a vanishing intrinsic FM anisotropy, assuming $J_{\text{int}}/J_{\text{FM}} = 0.4$. Evidently, $K_{\text{tot}}(T)$ 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 $K_{\text{tot,FM}}(T)$ is approximately given by the sum of $K_{\text{int}}(T)$ and $K_{\text{FM}}(T)$, see the dot-dashed line (c). Finally, by assuming $K_{\text{FM}}/J_{\text{FM}} = -0.01$ the dotted line (d) refers to the case of an intrinsic FM anisotropy favoring the same easy axis than $K_{\text{int}}$. Therefore, the absolute value $|K_{\text{tot,FM}}(T)|$ may be either reduced (c) or enhanced (d) by the interlayer exchange coupling. We emphasize that for the former case the two anisotropies $K_{\text{FM}}(T)$ and $K_{\text{int}}(T)$ compete, resulting possibly in a change of sign of $K_{\text{tot,FM}}(T)$, 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 $K_{\text{tot,FM}}(T)$ for different values of the interlayer exchange coupling $J_{\text{int}}$ and for the FM film thickness $n_{\text{FM}} = 5$. Furthermore, Fig.3 shows $K_{\text{tot,FM}}(T)$ for different $n_{\text{FM}}$, assuming $J_{\text{int}}/J_{\text{FM}} = 0.4$. The cho-

FIG. 1: Total effective anisotropy $K_{\text{tot,FM}}(T)$ per spin of the FM film as a function of temperature $T$. $K_{\text{tot,FM}}(T) > 0$ prefers a collinear, and $K_{\text{tot,FM}}(T) < 0$ an orthogonal FM film magnetization with respect to the AFM magnetic direction. The exchange couplings, intrinsic anisotropies, and temperatures are given in units of $J_{\text{FM}}$, and $K_{\text{tot,FM}}(T)$ in units of $K_{\text{FM}} = K_{\text{FM}}(T = 0)$. We assume $J_{\text{AFM}}/J_{\text{FM}} = -0.5$ and $K_{\text{AFM}}/J_{\text{FM}} = 0.01$, in addition $n_{\text{FM}} = 5$ and $n_{\text{AFM}} = 10$ for the thicknesses of the FM and AFM films. For these values the Curie temperature $T_C$ of the FM film is larger than the Néel temperature $T_N$ of the AFM film. The full line (a) shows the intrinsic anisotropy for a decoupled FM film ($J_{\text{int}} = 0$) for $K_{\text{FM}}/J_{\text{FM}} = 0.01$. The dashed line (b) refers to the bare interface anisotropy ($K_{\text{FM}} = 0$), assuming $J_{\text{int}}/J_{\text{FM}} = 0.4$. The presence of both anisotropic contributions results in a reduced $K_{\text{tot,FM}}(T)$, dot-dashed line (c). For $K_{\text{FM}}/J_{\text{FM}} = -0.01$ an enhanced absolute value $|K_{\text{tot,FM}}(T)|$ is obtained, dotted line (d).
sen parameters yield $T_C > T_N$. As mentioned, $K_{FM}$ favors an easy axis collinear to the AFM magnetization. $K_{tot,FM}(T)$ changes sign at the reorientation temperature $T_R$ for a strong $J_{int}$ or for a small $n_{FM}$. 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 $\phi_{0,FM}$, which are also depicted in Figs.2.3. We emphasize that the orthogonal arrangement ($\phi_{0,FM} = \pi/2$) 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 $0 < \phi_{0,FM} < \pi/2$. In this case the free energy $F(T, \phi_{FM})$ as a function of $\phi_{FM}$ exhibits four minima rather than two as for a simple uniaxial anisotropy. A two-fold symmetry is still present. For very strong $J_{int}$ also hysteresis effects may occur by varying $\phi_{FM}$, accompanied by sudden jumps of the AFM spin angles $\phi_i$ (spin-flop-transition). The AFM film exhibits a noncollinear, spin-flop-like magnetic arrangement for $\phi_{0,FM} > 0$. 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 $|K_{tot,FM}(T)|$ may occur, corresponding to a very soft ferromagnet. We note that $K_{tot,FM}(T)$ does not depend on the sign of $J_{int}$, consistent with the estimate $K_{int} \propto -(J_{int})^2/|J_{AFM}|$. The disturbance of the AFM spins in the spin-flop-phase decreases rapidly with increasing distance from the interface.

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 $K_{tot,FM}(T)$ is shown in Fig.4 for different interlayer exchange couplings $J_{int}$. By assuming $n_{FM} = 1$ and $J_{AFM}/J_{FM} = -0.75$, we obtain $T_C/J_{FM} = 2.47$ and $T_N/J_{FM} = 2.90$. 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 $K_{int}(T)$ is induced in the FM film, resulting in an orthogonal magnetic arrangement. For $T < T_C$ the intrinsic FM anisotropy $K_{FM}(T)$ becomes increasingly important and may cause a magnetic reorientation into the collinear arrangement with a decreasing temperature. Furthermore, an intermediate value of $J_{int}$ 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 $\phi_{0,FM}$, which is also shown in Fig.4 for $J_{int}/J_{FM} = 0.2$. A continuous variation of $\phi_{0,FM}$ 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 $J_{int}$ 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 $J_{int}$ by applying an external magnetic field, inducing a spin-flop transition in the AFM subsystem. However, to create such a spin-flop transition the magnetic field must possibly be very strong. We propose that $J_{int}$ can be determined by measuring the total anisotropy $K_{tot,FM}(T)$ 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 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.
FIG. 4: Total effective anisotropy $K_{\text{tot,FM}}(T)$ per FM film spin as a function of temperature for different interlayer exchange couplings $J_{\text{int}}$, assuming $n_{\text{FM}} = 1$ and $J_{\text{AFM}}/J_{\text{FM}} = -0.75$. For these values one obtains $T_G < T_N$. The equilibrium angle $\phi_{0,\text{FM}}(T)$ of the FM film magnetization is shown for $J_{\text{int}}/J_{\text{FM}} = 0.2$. For this value a reentrant magnetic behavior is obtained, indicated by changes of sign of $K_{\text{tot,FM}}(T)$ near the reorientation temperatures $T_R$, and a hysteresis close to $T_G$.

roughness, defects, and noncompensated AFM spins, accompanied possibly by a domain phase in the AFM subsystem. In the actual study this phenomenon has not been addressed.

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 $J_{\text{int}}$ causes an interface anisotropy $K_{\text{int}}(T)$, which adds to the intrinsic anisotropy $K_{\text{FM}}(T)$ of the FM film, and vanishes above the Neél temperature $T_N$ of the AFM system. Depending on the sign of $K_{\text{FM}}(T)$, the total anisotropy $K_{\text{tot,FM}}(T)$ of the FM film may be enhanced as well as 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 $n_{\text{FM}}$, 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 $K_{\text{FM}}(T)$ and $K_{\text{int}}(T)$. The magnetizations of the FM and AFM films can be either collinear or orthogonal to each other. In addition a canting magnetic arrangement may occur. Hence, the assumption that the magnetic structures in coupled FM-AFM systems are either collinear or orthogonal is not always true. The non-collinear, spin-flop-like arrangement of the AFM spins is vanishingly small for $\phi_{0,\text{FM}} > 0$ with increasing distance from the FM-AFM interface.

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$K_{\text{tot,FM}}(T) / K_{\text{FM}}(0)$

- (a) $J_{\text{int}} = 0.0$  
  $K_{\text{FM}} = 0.01$

- (b) $J_{\text{int}} = 0.4$  
  $K_{\text{FM}} = 0.0$

- (c) $J_{\text{int}} = 0.4$  
  $K_{\text{FM}} = 0.01$

- (d) $J_{\text{int}} = 0.4$  
  $K_{\text{FM}} = -0.01$

$n_{\text{FM}} = 5$

$T_C$

$T_N$

Temperature $T / J_{\text{FM}}$

Temperature $T$
Fig. 2
Fig. 3

\[ \frac{J_{\text{int}}}{J_{\text{FM}}} = 0.4 \]

\[ K_{\text{tot,FM}} / K_{\text{FM}}(0) \]

\[ \phi_{0,\text{FM}} \text{ [deg]} \]

\[ \text{temperature } T / J_{\text{FM}} \]

- \( n_{\text{FM}} = 2 \)
- \( n_{\text{FM}} = 3 \)
- \( n_{\text{FM}} = 5 \)
- \( n_{\text{FM}} = 8 \)
Fig. 4

$T_C$, $T_N$

$K_{tot,FM}(T) / K_{FM}(0)$

$\phi_{0,FM}(T) [\text{deg}]$

$J_{int} = 0.16$
$J_{int} = 0.18$
$J_{int} = 0.20$
$J_{int} = 0.22$

$n_{FM} = 1$

Temperature $T / J_{FM}$