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Exchange bias due to configurational magnetic rearrangements

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By considering collinear and noncollinear magnetic configurations the interlayer exchange energy can be viewed as a continuous energy parameter ϵ that can directly be correlated with the magnetoresistance. It is shown for the spin-valve system Co(111)/Co_6/$(CoO)_n$/Co_6/Cu_6/Co_6/Co(111), $n=6,12$, that the exchange bias refers to that value of ϵ below which the magnetoresistance remains zero. Above this value a gradual change in the magnetoresistance is observed when considering noncollinear magnetic configurations. All calculations are performed in terms of the fully relativistic spin-polarized versions of the screened Korringa-Kohn-Rostoker method and the Kubo-Greenwood equation.

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In a recent paper[1] the phenomenology of exchange bias and related effects with emphasis on layered ferromagnetic-antiferromagnetic (FM-AFM) structures is reviewed. Such an exchange bias occurs when systems with FM-AFM interfaces are cooled through the Néel temperature (T_N) of the AFM part, whereby the Curie temperature (T_C) of the FM part has to be larger than T_N. After the field cool procedure, at a temperature $T<T_N$, the hysteresis loop of the FM-AFM system is shifted along the field axis generally in the opposite direction of the cooling field, i.e., the absolute value of the coercive field for decreasing and increasing field is different. This loop shift is usually termed exchange bias and was found and investigated in quite a few different experiments such as magnetization and magnetic torque measurements, ferromagnetic resonance, neutron diffraction, magnetoresistance, etc.,[1] FM-AFM structures are presently very much under discussion as they seem to be of enormous importance for magnetic recording and related devices.

Up to now, however, only phenomenological or semiclassical models, see, e.g., Ref. 2, are in use in order to explain exchange bias effects. In here an attempt is made to head for a microscopical (*ab initio* type, no adjustable parameters) description of exchange biased spin-valve systems by simultaneously considering interlayer exchange energies and the magnetoresistance (MR) in the current-perpendicular to the planes (CPP) and current-in-plane (CIP) geometries.

Usually in terms of the magnetic force theorem the interlayer exchange coupling energy $\Delta E(C_i)$ is defined[3,4] as the difference in the single particle grand canonical potentials $E(C_i)$ between two (collinear) magnetic configurations

$$\Delta E(C_i)=E(C_i)-E(C_1), \tag{1}$$

where C_1 is a given reference magnetic configuration and C_i a magnetic configuration in which the orientation of the magnetization in a certain subset of atomic layers is reversed with respect to C_1. In a similar manner one can define the MR for perpendicular electric transport as a weighted difference in sheet resistances (resistivities in the case of CIP) $r(C_i)$ between these two (prechosen) magnetic configurations

$$R(C_i)=\frac{r(C_1)-r(C_i)}{r(C_1)}. \tag{2}$$

Suppose that for a two-dimensional translational invariant system (layered system) a particular configuration $C_i=\{\ldots,n_{k-1},n_k,n_{k+1},\ldots\}$, where k numbers atomic layers, is defined[5] by a set of collinear unit vectors n_k that characterize the orientations of the magnetization in all atomic layers considered, then configuration $C_j=\{\ldots,n_{k-1},-n_k,n_{k+1},\ldots\}$ refers to an arrangement in which with respect to C_i the orientation of the magnetization is reversed in the kth atomic layer. Taking also noncollinear configurations into account implies that C_j can be reached[5] in a continuous manner by means of a rotation $U(\Theta)$ of n_k, $0\leqslant\Theta\leqslant 2\pi$, around an axis perpendicular to n_k, i.e., by considering configurations of the form $C_i(\Theta)=\{\ldots,n_{k-1},U(\Theta)n_k,n_{k+1},\ldots\}$. Clearly enough in such a case the interlayer exchange energy $\Delta E[C_i(\Theta)]=E[C_i(\Theta)]-E[C_i(0)]$ varies continuously[6] from zero to $E(C_j)-E(C_i)$.

If C_1 denotes the (collinear) ground state magnetic configuration then the interlayer exchange energy, see Eq. (1), can be viewed as a continuous variable $\epsilon\geqslant 0$ provided that also noncollinear configurations are taken into account. Suppose $\mathcal{C}$ denotes the set of all collinear magnetic configurations then the set of corresponding interlayer exchange energies simply consists of certain values of ϵ that can be ordered according to magnitude.

In principle therefore one can view the MR as an implicit function of ϵ,

$$R(\epsilon)=\frac{r(C_1)-r(\epsilon)}{r(C_1)}, \tag{3}$$

where in CPP $r(\epsilon)$ is that sheet resistance (resistivity in the case of CIP) which (with respect to C_1) corresponds to a magnetic configuration of interlayer exchange energy ϵ. Clearly enough for certain regimes of ϵ the magnetoresistance $R(\epsilon)$ remains constant while in other regimes rapid changes with ϵ occur: the interlayer exchange energy ϵ acts as a magnetic field (external energy) that is switched on continuously. Increasing ϵ "forces" the system to gradually assume the magnetic configuration with the next highest en-

Co(111)		Θ	10	9	8	7	6	5	4	3	2	1
Co	1	0	0	0	0	0	0	0	0	0	0	0
Co	2	0	0	0	0	0	0	0	0	0	0	0
Co	3	0	0	0	0	0	0	0	0	0	0	0
Co	4	0	0	0	0	0	0	0	0	0	0	0
Co	5	0	0	0	0	0	0	0	0	0	0	0
Co	6	0	0	0	0	0	0	0	0	0	0	0
O	1	1	1	1	1	1	1	1	1	1	1	1
Co	1	1	1	1	1	1	1	1	1	1	1	1
O	2	0	0	0	0	0	0	0	0	0	0	0
Co	2	0	0	0	0	0	0	0	0	0	0	0
O	3	1	1	1	0	1	1	1	1	1	1	0
Co	3	1	1	1	1	1	1	1	1	1	1	1
O	4	0	0	0	0	0	0	0	0	0	0	0
Co	4	0	0	0	0	0	0	0	0	0	0	0
O	5	1	1	0	0	1	1	1	1	1	0	0
Co	5	1	1	1	1	1	1	1	1	1	1	1
O	6	0	0	0	0	0	0	0	0	0	0	0
Co	6	0	0	0	0	0	0	0	0	0	0	0
Co	1	0	0	0	0	0	0	0	0	0	0	0
Co	2	0	0	0	0	0	0	0	0	0	0	0
Co	3	0	0	0	0	0	0	0	0	0	0	0
Co	4	0	0	0	0	0	0	0	0	0	0	0
Co	5	0	0	0	0	0	0	0	0	0	0	0
Co	6	0	0	0	0	0	0	0	0	0	0	0
Cu	1	0	0	0	0	0	0	0	0	0	0	0
Cu	2	Θ	0	0	0	1	0	0	0	0	0	0
Cu	3	Θ	0	0	0	1	0	1	0	0	0	0
Cu	4	Θ	0	0	0	1	0	1	0	1	1	1
Cu	5	Θ	0	0	0	1	0	1	1	1	1	1
Cu	6	Θ	0	0	0	1	1	1	1	1	1	1
Co	1	Θ	0	0	0	1	1	1	1	1	1	1
Co	2	Θ	0	0	0	1	1	1	1	1	1	1
Co	3	Θ	0	0	0	1	1	1	1	1	1	1
Co	4	Θ	0	0	0	1	1	1	1	1	1	1
Co	5	Θ	0	0	0	1	1	1	1	1	1	1
Co	6	Θ	0	0	0	1	1	1	1	1	1	1
Co(111)												

FIG. 1. Magnetic configurations: configuration C_{10} was used for matters of self-consistency. Configurations $C_1 - C_{10}$ lead to the ten lowest interlayer exchange energies. Zero (one) indicate that in a particular layer the orientation of the magnetization is parallel (antiparallel) to the surface normal. Θ varies between zero and 180° and leads continuously and uniformly from C_7 to C_{10}.

ergy, etc. Consequently one can define the exchange bias E_{bias} in terms of $R(\epsilon)$ in the following manner;

$$0 \leq \epsilon \leq E_{\mathrm{bias}} : R(\epsilon) = 0; \epsilon > E_{\mathrm{bias}} : R(\epsilon) \neq 0. \tag{4}$$

Obviously for all $\epsilon \leq E_{\mathrm{bias}}$ it is sufficient to consider only collinear configurations, while for $\epsilon > E_{\mathrm{bias}}$ also particular noncollinear configurations have to be taken into account. It should be noted that of course this definition applies only to systems for which a recordable change in the MR can be observed, e.g., in spin-valve systems with an AF part.

In here the fully relativistic spin-polarized screened Korringa-Kohn-Rostoker method for layered systems[3,4] is applied to calculate the electronic structure and magnetic properties of $Co(111)/Co_6/(CoO)_n/Co_6/Cu_6/Co_6/Co(111)$, $n = 6,12$. In all calculations an fcc-Co parent lattice[5] is assumed with a lattice spacing a_0 of 6.5509 a.u. (bulk fcc Co), i.e., no layer relaxation is considered, and six Co layers serve as buffer to the semi-infinite leads. In order to determine selfconsistently within the local density approximation[7] (LDA) the effective potentials and effective exchange fields a minimum of 45 $\mathbf{k}_{\parallel}$ points in the irreducible wedge of the surface Brillouin zone (ISBZ) was used. All selfconsistent calculations refer to the "antiferromagnetic" configuration C_{10} listed in Fig. 1, all interlayer exchange energies are evaluated by using a total of 990 $\mathbf{k}_{\parallel}$ points in the ISBZ, which—as was shown[4] in the case of magnetic anisotropy energies—guarantees well converged results. All electric transport calculations were performed in terms of the

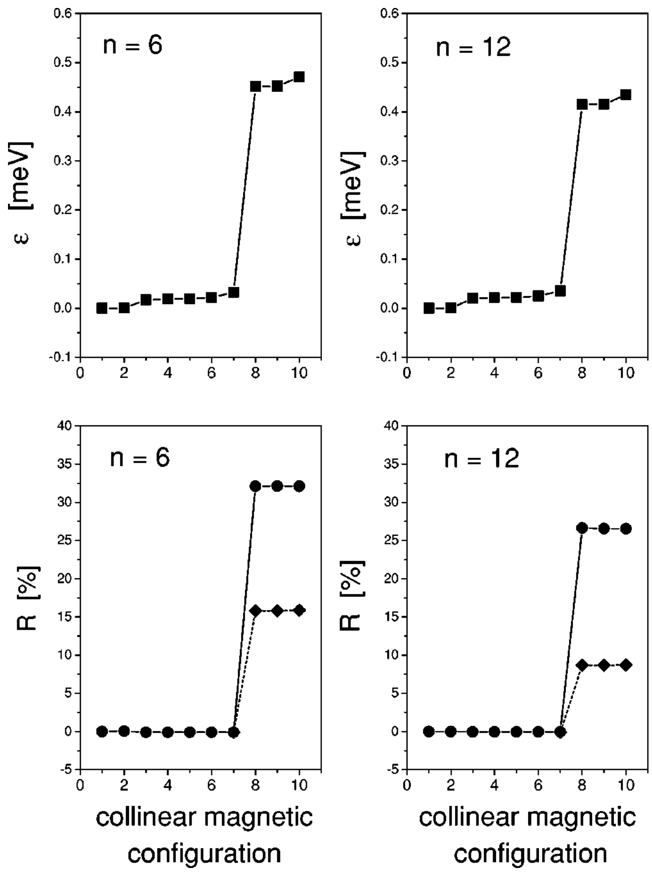

FIG. 2. The ten lowest interlayer exchange energies and corresponding magnetoresistances. CPP and CIP are denoted by circles and diamonds, respectively. The number of repetitions of a CoO double layer is marked explicitly.

fully relativistic spin-polarized form of the Kubo-Greenwood equation for layered systems[8,9] by using a complex Fermi energy and 1830 $\mathbf{k}_{\parallel}$ points in the ISBZ for the SBZ integrals, and by continuing the thus obtained sheet resistances[10] (resistivities in the case of CIP) numerically to the real energy axis. In order to find the lowest excited collinear states for a total of 45 different collinear magnetic configurations the interlayer exchange energy and the magnetoresistance was evaluated considering collinear "spin flips" not only in the CoO part of the system, but also in the Co slabs and in the Cu spacer. It should be noted that for six Cu layers antiferromagnetic coupling between the two FM Co slabs pertains.[6,11]

In Fig. 1 those collinear magnetic configurations referring to the ten smallest interlayer exchange energies with respect to configuration C_1 (ground state) are displayed for $n=6$. For $n=12$ the second half of the CoO part of the systems is analogous to configuration C_{10} in Fig. 1. In Fig. 2 the corresponding interlayer exchange energies and MR (CIP and CPP) are shown for $n=6$ and 12. Although the interlayer exchange energy increases for the first seven (collinear) configurations the MR remains zero and only jumps suddenly between configuration C_7 and C_8. This jump between configurations C_7 and C_8 is characteristic for both thicknesses of the CoO part of the system. Figure 3 resolves this sudden

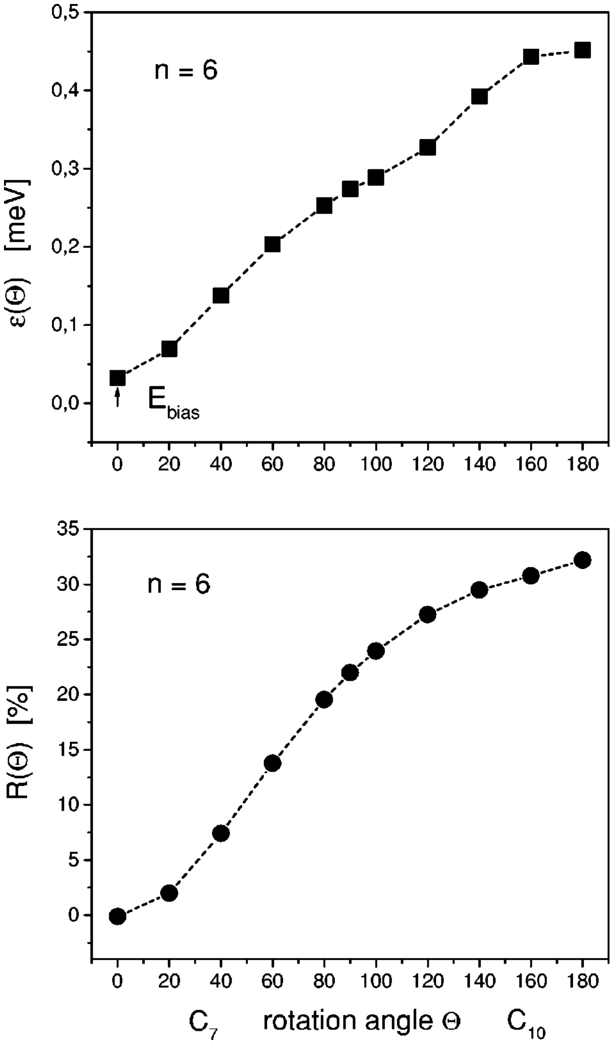

FIG. 3. Interlayer exchange energy and CPP magnetoresistance as a function of the rotation angle Θ for a rotation around the *y* axis. The two collinear magnetic configurations that correspond to the end points are marked explicitly.

jump in terms of a continuous rotation, i.e., by going continuously from configuration C_7 to configuration C_{10} by means of the noncollinear configurations headed by "Θ" in Fig. 1. From Fig. 3 one can see that the interlayer exchange energy $\epsilon(\Theta)$ and $R(\Theta)$ indeed vary continuously but also that because of relativistic effects $\epsilon(\Theta)$ differs considerably from a functional form[6] that is proportional to $\frac{1}{2}[1-\cos(\Theta)]$. In Fig. 4 $R(\epsilon)$ versus ϵ is shown for $n=6$. In here collinear magnetic configurations refer to full symbols whereas noncollinearity between configurations C_7 and C_{10} is displayed in terms of open symbols: on the scale of ϵ shown in this figure the exchange bias constitutes just the very beginning of this curve. In general the "flip energy" E_{flip} that causes the jump in the MR can be defined as the difference between E_{bias} and the closest larger collinear interlayer exchange energy (C_8 in the present case). In the present case this energy amounts to 0.416 meV for $n=6$ and 0.399 meV for $n=12$. In order to give a rough estimate in kOe, by using the relation $\Delta E=\mu_B B$ (1 meV=172.76 kOe), these energies amount to 72 and 69 kOe, respectively.

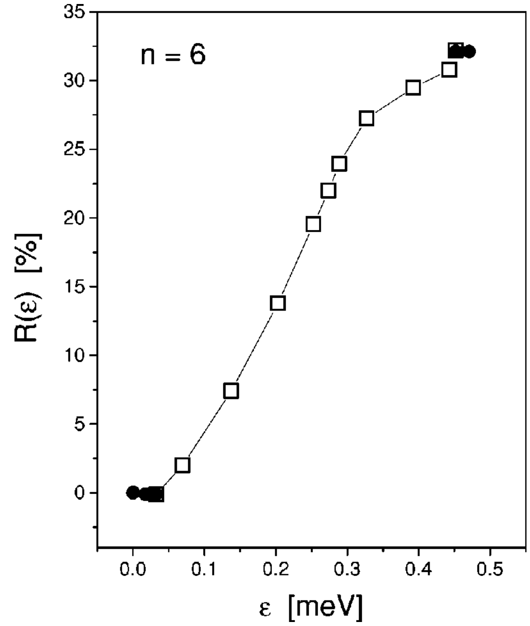

FIG. 4. CPP magnetoresistance for $n=6$ as a function of the interlayer exchange energy. Collinear magnetic configurations are shown in terms of full symbols.

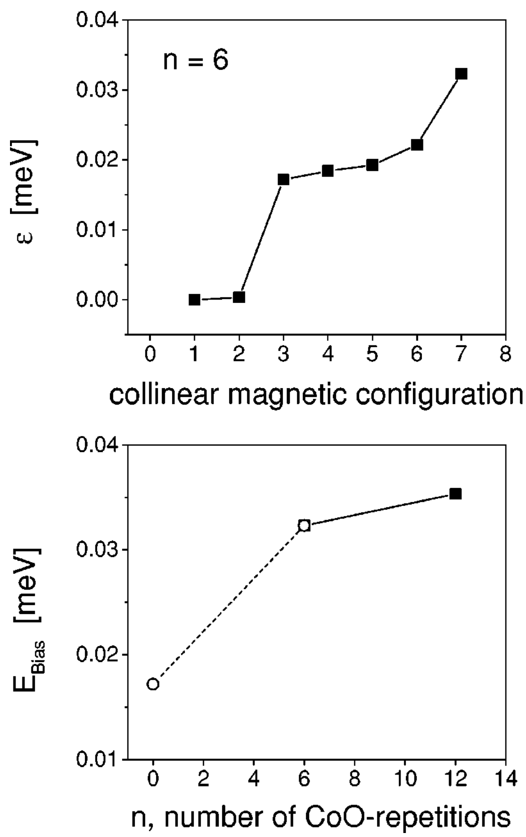

FIG. 5. Top: Interlayer exchange energy $\epsilon \leq E_{\mathrm{bias}}$ for $n=6$. Bottom: Exchange bias as a function of the number of repetitions of a CoO double layer. The value at $n=0$ (open symbol) is an extrapolation, see text.

E_{bias} is caused by two different types of effects, namely, (1) a rearrangement of the orientations of the magnetization in the oxygen layers and (2) a rearrangement of orientations in the Cu spacer layers. This can be seen best by replotting the interface energy for $\epsilon \leqslant E_{bias}$. From Fig. 5 (top) it is obvious that about half of E_{bias} arises from the rearrangement of orientations in the Cu spacer layers. For $n \geqslant 6$ E_{bias} depends only very weakly on the thickness of the CoO part of the system and amounts to about 0.035 meV (6 kOe, see above relation), which seems to be in reasonably good agreement with the experimental values ($E_{bias} \leqslant 9.5$ kOe) reported[1] for Co/CoO type systems. Using the value of C_3 from the top part of Fig. 5, it is tempting to extrapolate to the case of $n=0$, i.e., to a complete absence of the AFM part of the system. As can be seen from Fig. 5 (bottom) E_{bias} would then drop substantially, which in turn is very much in line with experimental evidence.[1] Increasing the interlayer exchange energy ϵ, $E_{bias} \leqslant \epsilon \leqslant (E_{bias}+E_{flip})$, in terms of noncollinear configurations eventually leads to a reversed orientation of the magnetization in that Co slab that does not form the interface with the AFM part of the system, see also Fig. 1. This particular behavior is the microscopic reason for using AFM parts as ''pinning layers.''

Quite clearly in an actual system of the type Co(111)/$(CoO)_n/Co_{t_1}/Cu_s/Co_{t_2}$/Cap the exchange bias not only depends on all relevant thickness parameters, namely, n, t_1, t_2, and s, the thickness of the AFM CoO layer, the FM Co layers, the Cu spacer and the type, and thickness of the cap, but also on the actual layer distances and the quality of the various interfaces present in such a system. However, all these effects are discussed at length from an experimental standpoint of view in the review paper by Nogués and Schuller,[1] and references therein. In here the main emphasis was put on the microscopical origin of the exchange bias, at least as viewed in terms of the MR for a model spin-valve system containing AF parts, of course omitting all possible dynamical effects. From Fig. 2 follows that the definition of the exchange bias in terms of Eq. (4) is independent of the type of MR (CIP or CPP) to be correlated with the interlayer exchange energy.

In summary it can be said that the exchange bias in spin-valve systems with FM-AFM interfaces very likely is caused mainly by configurational magnetic rearrangements in the nonmetal parts of the AFM subsystem and in the (''nonmagnetic'') metal spacer parts. A description of this phenomenon based on *ab initio* calculations such as presented in here, however, can only be given by considering simultaneously two quantities, namely an appropriate energy variable, e.g., the interlayer exchange energy, and a physical property by which—similar to experiment—the alignments in the FM parts of a given system can be monitored.

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