Helimagnetism and competition of exchange interactions in bulk giant magnetoresistance alloys based on $MnAu_2$

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By using the generalized perturbation method within the screened Korringa-Kohn-Rostoker formalism we calculate magnetic exchange interactions in the helimagnetic bulk $MnAu_2$ compound upon alloying Mn with Fe and Cr. The obtained interactions reproduce well the results of neutron diffraction experiments concerning the periodicity of the helix in $MnAu_2$ and its weakening with Fe substitution thus supporting the conventional interpretation of a metamagnet-ferromagnet transitions due to external fields. In the case of $Mn_{1-x}Cr_xAu_2$ alloys our results reveal that the experimentally observed magnetization process follows a completely different scenario, predicted theoretically a few decades ago for nearly orthogonal helimagnetics.

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I. INTRODUCTION

Intense studies of metamagnetic transitions in systems with complex magnetic ordering have significantly extended our knowledge about solid state magnetism beyond simplified models of collinear ferromagnetism. After the discovery of giant magnetoresistance (GMR) in magnetic multilayers systems,[1,2] it has also been widely realized that sharp changes in physical properties such as electrical resistivity and magnetization of bulk materials caused by metamagnetic transitions have an enormous potential for technological applications. As an example, the familiar metamagnetic properties of the FeRh compound[3] has recently been exploited to generate ultrafast magnetic switching in electronic devices.[4] It has been shown also that some metamagnetic bulk materials with layered crystal structure and antiferromagnetic-like interlayer ordering in the ground state exhibit a strong GMR effect, which may be of the same origin as in metallic multilayers systems with antiferromagnetic interlayer coupling.[5] Such compounds may have obvious advantages for technological applications due to simple preparation requirements as single phase and are well suited for intensive experimental and theoretical studies of the GMR effect in general. At present, the body-centered-tetragonal $MnAu_2$ for which a pronounced GMR effect at room temperature was reported by Samata *et al.*,[6] is considered to be one of the most promising materials of this kind. In $MnAu_2$ the ferromagnetic basal planes of Mn atoms are separated by two layers of Au, thus forming a perfect multilayer superstructure. It is therefore quite natural to expect that the mechanism leading to the pronounced GMR effect in this system is of the same origin as in artificial multilayer superstructures.

The compound $MnAu_2$ was among the first systems for which the phenomenon of helimagnetic ordering, predicted theoretically by Yoshimori,[7] Villain,[8] and Kaplan,[9] was observed by neutron diffraction experiments.[10] In an applied magnetic field of $H \sim 1.5-2$ T, this compound exhibits a first order metamagnetic phase transition from a helical spin "screw" configuration to a "fan" like magnetic structure.[6,10] The threshold field, H_t, of this metamagnetic phase transition should clearly be distinguished from the critical field, H_c, at which the system becomes fully magnetized. In order to reduce H_t to values suitable for practical applications of the GMR effect, a partial replacement of the Mn atoms by other TM elements, like Cr,[11] Fe, and Co (Ref. 12) was tried. Magnetization measurements of such $Mn_{1-x}TM_xAu_2$ systems[11,12] indeed revealed decreasing threshold fields with increasing x, while preserving a GMR of similar order as in pure $MnAu_2$. There were, however, some differences observed between the Fe and Cr doped alloys. In $Mn_{1-x}Fe_xAu_2$ the low temperature threshold field decreases very fast with Fe doping such that already for $x_{Fe}=0.075$ the low temperature ground state is ferromagnetic,[13] whereas in $Mn_{1-x}Cr_xAu_2$ the estimated threshold field decreases only from $H_t \simeq 1.6$ T at $x_{Cr}=0$ to $H_t \simeq 0.8$ T at $x_{Cr}=0.15$ (Ref. 11) (see also the earlier measurements by Adachi *et al.*[14]). In addition, the high-field magnetization in $Mn_{0.85}Cr_{0.15}Au_2$ is approximately twice as small as in pure $MnAu_2$. This is in sharp contrast to the Fe doped case, where the saturation magnetization is even larger than in pure $MnAu_2$. So far, the observations in both cases have been discussed[11,12] in terms of a weakening of the interplane exchange coupling between the Mn moments caused by the TM substitution and a corresponding decrease of the energy of the spin-spiral configuration with respect to the ferromagnetic alignment.

In this paper we present first principles calculations of the electronic structure and the exchange interactions in pure $MnAu_2$ and of $Mn_{1-x}TM_xAu_2$ with TM=Fe and Cr. Our aim is thus to provide a microscopical background of the conventional phenomenological picture of helimagnetism and metamagnetism in $MnAu_2$ based systems and to explore the role played by TM substitutions in reducing the metamagnetic threshold field. As we will show, our results suggest an entirely novel interpretation of the metamagnetic process in $Mn_{1-x}Cr_xAu_2$ alloys.

II. CONVENTIONAL THEORY OF HELIMAGNETIMS

A theoretical description of metamagnetic transitions in helical structures was given in the framework of a Heisen-

berg model by Herpin and Meriel[10] and later elaborated by Enzl[15] and Nagamiya *et al.*[16] Within this model the magnetic energy is defined as

$$E = -\frac{1}{2}\sum_{i\neq j} J_{ij}\vec{e}_i\vec{e}_j - \vec{H}\sum_i \vec{M}_i, \tag{1}$$

where $\vec{M}_i$ is the magnetic moment at site i, $\vec{e}_i = \vec{M}_i/|\vec{M}_i|$, J_{ij} are exchange coupling constants, and $\vec{H}$ is an applied external field. In helimagnetic systems like $MnAu_2$ strong ferromagnetic coupling is assumed inside each layer of the magnetic atoms ensuring that at $T=0$ K all moments within one layer point in one direction. Defining thus an effective in-plane coupling constant, J_0, and interplane coupling constants, J_n, between the nth nearest-neighbor planes as a sum over pairs in the corresponding layers, one can write the magnetic energy in the absence of the external field as[16]

$$E/N = -\frac{L}{2}J_0 - J_1\sum_k \cos(\Delta\,\vartheta_{k+1,k}) - J_2\sum_k \cos(\Delta\,\vartheta_{k+2,k}) - \ldots, \tag{2}$$

where $\Delta\,\vartheta_{k+n,k}$ is the relative angle of the moments in the $k+n$th and the kth layers, L is the number of planes, and N is the total number of sites in a plane. Since for a helical spin-spiral configuration

$$\Delta\,\vartheta_{k+n,k} = n\varphi \quad (\forall k,n), \tag{3}$$

the energy per magnetic atom can be expressed as

$$E(\varphi) = -\frac{1}{2}J_0 - J_1\cos(\varphi) - J_2\cos(2\varphi) - \ldots, \tag{4}$$

that has to be minimized with respect to the angle φ. Thus a spin spiral with a finite angle, φ, can be stabilized by the competition of the interplane interactions, J_i, of different signs. The minimum value of the external field, H_c, needed to turn the system into a collinear ferromagnetic state is directly provided by the energy difference between the ferromagnetic state and the spin-spiral state as characterized by the angle, φ,

$$H_cM = E(\varphi=0) - E(\varphi) = \Delta E(\varphi) = J_1[\cos(\varphi)-1] + J_2[\cos(2\varphi)-1] + \ldots. \tag{5}$$

In applied external fields, $0<H<H_c$, a general description of the magnetization processes in helimagnetic systems exhibits a nontrivial mathematical problem that can be solved only approximately.[15] Here we just outline the main results derived in Refs. 10, 15, and 16 which we shall use in the present paper. In low applied fields the magnetic moments of the ferromagnetic layers tend to tilt towards the field direction and the resulting structure can be viewed as a deformed helix, in which the original spin spiral is slightly modulated by small sinusoidal oscillations. If the external field is applied parallel to the ferromagnetic planes (perpendicular to the helix propagation vector), or there is a strong easy plane magnetic anisotropy as in the case of $MnAu_2$, the magnetic configurations remains a proper screw with all moments oriented within the planes. At the threshold field, H_t, a first-order phase transition occurs from the screw to a "fan" structure. In the fan or sine-wave phase the orientations of the moments in all planes make a sharp angle with the direction of the applied field and they oscillate sinusoidally around it. A schematic representation of this conventional scenario is given in Fig. 1(a). It should be noted that in an ideal single crystal the magnetization saturates only for fields higher than H_c; for fields close to H_t it is far from full saturation. The analysis given, e.g., in Ref. 16, has shown that the exact value of H_t depends on the angle of the original spin spiral, whereas this dependence is very moderate, since generally $0.414\,H_c < H_t < 0.5\,H_c$. Herpin and Meriel[10] found that for $MnAu_2$ $H_t = 0.485\,H_c$. Since H_c, as defined by Eq. (5), becomes smaller as the spin spiral weakens, for a decreasing spin spiral angle the metamagnetic threshold field, H_t, also decreases.

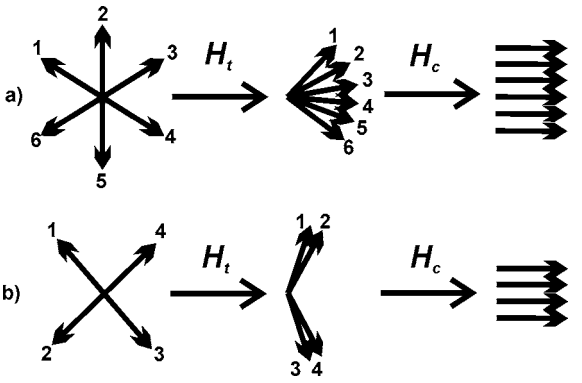

FIG. 1. Sketch of the metamagnetic transitions in helical structures due to an applied external field: (a) screw to fan transition (Refs. 10 and 15); (b) scenario for nearly orthogonal helical structures (Ref. 16). The numbers denote subsequent layers of magnetic atoms.

Assuming qualitatively near proportionality betwen H_t and H_c observed in pure $MnAu_2$, the outlined model seems to provide a sound interpretation of the experimentally observed decrease of H_t caused by Cr and Fe substitution of Mn in the $MnAu_2$ compound:[11,12] the substitution of Cr or Fe weakens (renormalizes) the interplane Mn-Mn interactions and, therefore, the spin-spiral angle decreases. Very recent neutron diffraction experiments[13] confirmed this scenario for the case of Fe substitution. It has been found that at low temperatures the wave vector, and, correspondingly, the angle of the helix decreases when the Fe concentration, x, increases in $Mn_{1-x}Fe_xAu_2$. The helical structure completely vanishes for alloys with $x>0.075$. To our best knowledge, there are no neutron diffraction studies for $Mn_{1-x}Cr_xAu_2$ alloys, but the magnetization processes in these systems has been interpreted[11,14] in a similar manner as for the Fe substitution. We will discuss in Sec. IV that the *ab initio* calculations suggest for this case a new kind of metamagnetic phase transition valid for nearly orthogonal helix structures.

III. COMPUTATIONAL DETAILS

The fully relativistic, spin-polarized screened Korringa-Kohn-Rostoker (SKKR) method for layered systems[17] as

TABLE I. Calculated magnetic moments in (μ_B), effective interlayer exchange coupling constants (mRy), and angles of the helical spin-spiral configurations in $Mn_{1-x}TM_xAu_2$ alloys (TM=Fe, Cr). Experimental angles were taken from Refs. 10 and 13.

Fe,Cr (at. %)	0	5% Fe	10% Fe	5% Cr	10% Cr
M_{Mn}	3.89	3.89	3.89	3.88	3.89
$M_{\mathrm{Fe,Cr}}$		3.27	3.27	3.06	3.06
J_0	10.352	9.477	8.676	11.165	11.853
J_1	1.849	1.899	1.950	1.410	0.786
J_2	−0.611	−0.462	−0.357	−0.757	−0.912
J_3	−0.076	−0.098	−0.095	−0.010	−0.117
φ calc.(exp.)	47 deg (∼51 deg)	37 deg (∼23 deg)	25 deg (0)	62 deg	83 deg

combined with the coherent potential approximation[18] (CPA) is applied to calculate the electronic structure and magnetic properties of $Mn_{1-x}TM_xAu_2$ systems. All calculations have been performed at the experimental lattice constant[12] of the bct structure of $MnAu_2$. The effective potentials and exchange fields have been determined selfconsistently within the local density approximation[19] (LDA) and by using the atomic sphere approximation (ASA). In order to perform energy integrations 12 energy points along a semicircular contour in the upper complex plane have been used and, at each energy point, a total of 36 k points in the irreducible wedge of the surface Brillouin zone (ISBZ) was selected for the necessary BZ integration.

Subsequent to the selfconsistent calculations, the exchange couplings, J_{ij}, were calculated by using a relativistic extension[21] of the torque method.[20] Note that only the isotropic part of the exchange interactions has been considered in the present work. In order to ensure a sufficient numerical accuracy of the calculated J_{ij}'s the corresponding BZ integration was performed using 1860 $\mathbf{k}_\parallel$ points in the ISBZ at the energy closest to the Fermi level, while the number of k points was gradually decreased for energy points more distant from the real axis in the complex plane and toward the bottom of the band. In the case of chemical disorder, the exchange coupling between different components of the alloy were determined in the spirit of the generalized perturbation method (GPM), i.e., by neglecting vertex corrections, see, e.g., Ref. 22. The obtained, component specific, in-plane, and interlayer exchange coupling constants, $J_n^{\mathrm{Mn\text{-}Mn}}$, $J_n^{\mathrm{TM\text{-}TM}}$ and $J_n^{\mathrm{Mn\text{-}TM}}$, were then used to define effective exchange coupling constants

$$J_n = (1-x)^2 J_n^{\mathrm{Mn\text{-}Mn}} + 2x(1-x) J_n^{\mathrm{Mn\text{-}TM}} + x^2 J_n^{\mathrm{TM\text{-}TM}}. \quad (6)$$

IV. RESULTS AND DISCUSSION

The calculated magnetic moments, in-plane (J_0) as well as interplane (J_n) exchange constants, Eq. (6), are summarized in Table I. The moment of Mn (3.89 μ_B) is almost unaffected by the TM substitution. This value is slightly larger than the experimental estimate (3.5 μ_B) for pure $MnAu_2$.[6] This difference can be understood considering that the experimental Mn moment was estimated from a fit of the high field magnetizations to an infinite value of the applied field, whereby it was assumed that $MnAu_2$ in fields higher than H_t is in a ferromagnetic state and that the magnetization is given by its saturation value as in the case of a usual ferromagnet. However, as already mentioned, for fields $H_t < H < H_c$ $MnAu_2$ has a fan spin structure[10] in which the total magnetization is lower than in the ferromagnetic state [see Fig. 1(a)] and the magnetization shows a complex field dependence up to H_c. Using, therefore, for fitting magnetizations in external fields lower than H_c may cause an underestimation of the saturation magnetization. The moments of Fe and Cr are smaller than that of Mn, and, as can be seen from Table I, do depend only a little on the alloy composition.

The magnetic ground state of the system seems to correspond fairly well to the spin screw structure as depicted in Fig. 1(a). The calculated in-plane exchange constants J_0 suggest strong ferromagnetic coupling within the (100) layers of the bct structure, and are approximately five times larger than the ferromagnetic first nearest layer coupling constant J_1. The second nearest layer coupling constant J_2 is antiferromagnetic and its relatively large value as compared to J_1 leads to the stabilization of a helical spin spiral in $MnAu_2$. The third nearest layer interaction is also antiferromagnetic, although much smaller than the second one. However, it is strong enough to alter in $MnAu_2$ the spin-spiral angle by a few degrees and, therefore, it has to be taken into account in the following considerations. Note that for pure $MnAu_2$ we calculated a magnetic anisotropy energy of 1 meV/unit cell in size favoring an in-plane direction for the magnetization.

In Fig. 2 we plot the magnetic energy, Eq. (4), as a function of the helical angle as calculated from the J_i's given in Table I. The energy is given with respect to the collinear FM state. For $MnAu_2$ $\Delta E(\varphi)$ reaches a minimum at $\varphi=47$ deg which is in fair agreement with the experiment ($\varphi=51$ deg).[12,13] It can be seen in the upper panel of Fig. 2 that the angle of the helix decreases with an increasing Fe concentration, which is also in agreement with the trend observed in the neutron diffraction experiment for $Mn_{1-x}Fe_xAu_2$ alloys at low temperature.[13] With increasing Fe concentration $\Delta E(\varphi)$ drops very fast. Since the threshold field, H_t, is proportional to H_c,[16] our calculations also predict a fast decrease of H_t in $Mn_{1-x}Fe_xAu_2$ alloys, which is again in good agreement with experiments.[12,13] It should be noted, however, that at $T=5$ K the alloy with $x_{Fe}=0.1$ was found to

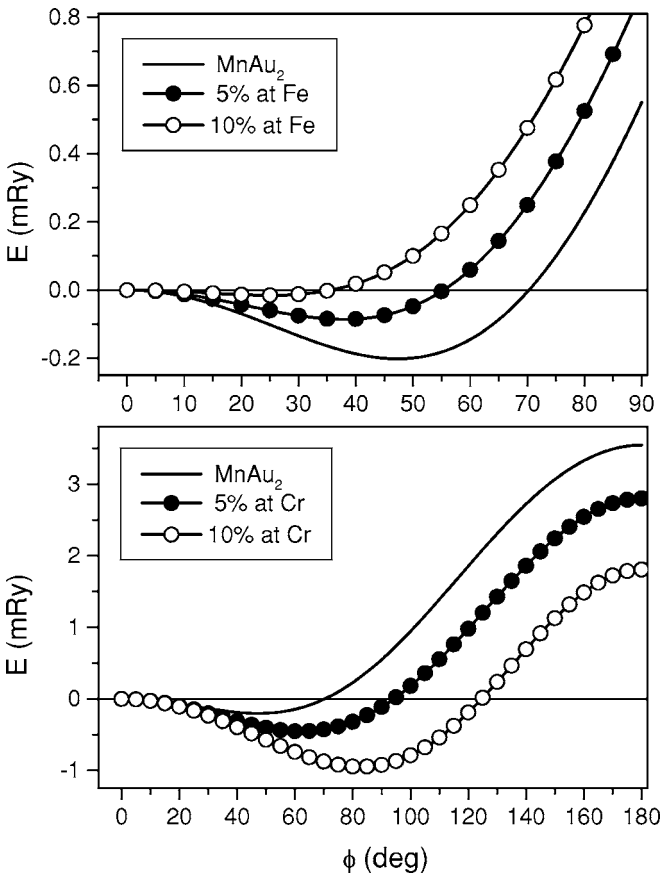

FIG. 2. Calculated energies of the helical structures with respect to the ferromagnetic phase for $Mn_{1-x}TM_xAu_2$ alloys (TM=Fe,Cr) as a function of the helix angle, φ.

be ferromagnetic, whereas our calculations predict a helical structure with a finite φ (see Table I and Fig. 2). Reassuringly, the energy difference between the FM and the helical structure becomes very small (0.015 mRy), i.e., falls into an energy range which is already beyond the conceptual accuracy of the LDA-GPM method.

Using the result of Herpin and Meriel[10] for $MnAu_2$, $H_t = 0.485\ H_c$, the calculated Mn moment from Table I and $\Delta E = 0.2$ mRy from Fig. 2 one can estimate the threshold field of the metamagnetic transition. The corresponding result $H_c = 6$ T is about three times larger than the experimental value (1.5–2 T).[6,10] It should be noted that any reliable quantitative estimate of realistic values for H_t, even in the case of an external field applied perpendicular to the direction of the helix, requires a knowledge of the in-plane magnetic anisotropy energy[16] which is, however, beyond the computational accuracy of our method.

At low temperatures a metamagnetic transition in $Mn_{1-x}Cr_xAu_2$ has been observed for all studied concentrations including $x_{Cr}=0.15$ (Ref. 11) suggesting that the helical configuration remains the ground state. The decrease of H_t has been interpreted as a weakening of the spin spiral upon Cr substitution and a corresponding decrease of its angle. Our results suggest just the opposite trend (see the lower panel of Fig. 2): the angle of the helical configuration increases and, simultaneously, the helical structure becomes energetically more stable with respect to the FM state. Our theoretical results are, therefore, not consistent with the conventional interpretation of a metamagnetic transition in these alloys as a screw to fan transition.

As can be seen from Table I and Fig. 2, the angle of the helix in the Cr doped case becomes close to 90 deg. For a nearly orthogonal helical structures Nagamiya *et al.*[16] pointed out that another kind of metamagnetic transition occurs, namely, a transition from the screw structure to a phase where the magnetic layers are partitioned into two sets: one comprising layers $n=1,2,5,6,\ldots$ and one comprising those for $n=3,4,7,8,\ldots$. The direction of the moments within each set is parallel to each other, and these two sets are tipped symmetrically with respect of the field directions. The schematic picture of such a transition is given in Fig. 1(b). The metamagnetic threshold field of such a transition drops very fast as the angle of the ground state helix approaches 90 deg, thus explaining the observed decrease of H_t in $Mn_{1-x}Cr_xAu_2$ alloys.

The results presented in Fig. 2 also explain why the magnetization of Cr doped alloys in an applied field of 5 T is much (nearly two times) smaller[11,14] than in pure $MnAu_2$. This happens because the helical structure becomes more stable and consequently H_c increases strongly upon Cr substitution. For the external fields used in the experiments the Cr doped alloys are much further away from the saturation than the pure $MnAu_2$. Note, that an opposite situation was found for the Fe doped alloys: the high field magnetization of $Mn_{0.95}Fe_{0.05}Au_2$ becomes even larger than the corresponding magnetization of pure $MnAu_2$.[12] These observations strongly support the validity of our results also for the Cr doped alloys. A direct experimental verification of such a novel scenario of metamagnetic transitions would require neutron diffraction experiments in order to directly answer the question of how the helix angle is changed at low temperatures upon increasing x in the $Mn_{1-x}Cr_xAu_2$ alloys.

The changes of the magnetic structure induced by TM substitutions in $MnAu_2$ can only be partially ascribed to the renormalization of the Mn-Mn exchange interactions. Both Fe and Cr have large moments (see Table I) and their exchange interactions with Mn contribute significantly to the effective exchange interactions, see Eq. (6). In order to obtain a better insight, in Fig. 3 we plot the contributions from Mn-Mn and Mn-TM pairs to the effective interplane coupling constants, J_1 and J_2, since the interplay of these interactions mainly determines the ground state of the helical configuration. Although comparable in magnitude, the TM-TM interactions are not plotted, since, due to a small concentration x, this part contributes only marginally to the effective coupling [consider the factor x^2 in Eq. (6)]. One can immediately note the different x dependence of $J_1^{\text{Mn-Mn}}$ for the Fe and Cr doped alloys: the substitution of Fe leads to a slight increase of the Mn-Mn coupling, whereas Cr leaves it almost unchanged. The main difference can, however, be seen in the Mn-Cr and Mn-Fe interactions: $J_1^{\text{Mn-Fe}}$ is by 10% larger than $J_1^{\text{Mn-Mn}}$. In addition, doping with Fe weakens the antiferromagnetic second nearest-plane Mn-Mn interaction $J_2^{\text{Mn-Mn}}$. All three facts mentioned above lead to a reduction of the energy of the spin-spiral configurations in $Mn_{1-x}Fe_xAu_2$ alloys as compared to the collinear FM state.

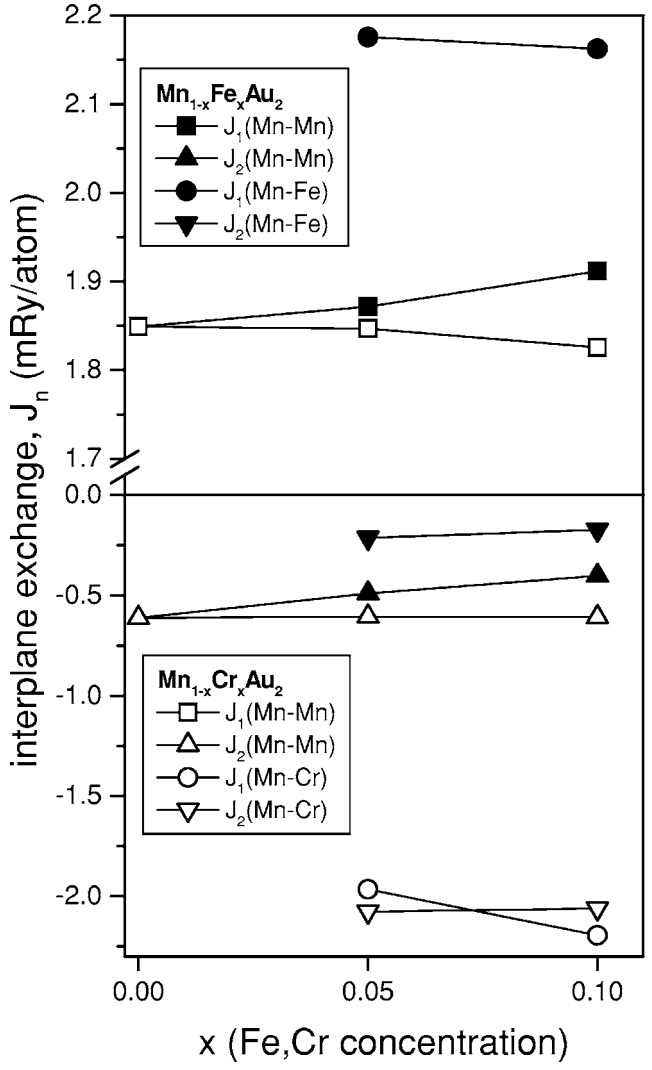

FIG. 3. Partial contributions to the effective interlayer exchange coupling, see Eq. (6), as a function of the concentration of the TM atoms x in $Mn_{1-x}TM_xAu_2$ alloys (TM=Fe,Cr).

The first and second nearest-plane Mn-Cr interactions, on the contrary, are both antiferromagnetic (AF) and similar in magnitude. Thus the strong AF Mn-Cr interactions drive the system towards antiferromagnetism by increasing the ground state helix angle and making the ferromagnetic (FM) state less favorable.

Our study concerns only the zero temperature case, however, some comments about finite temperatures have to be made. In all alloys studied the threshold field of the metamagnetic transition decreases with temperature.[11,12] In $Mn_{1-x}Fe_xAu_2$ some changes of the angle of the helix as a function of temperature were found from neutron diffraction measurements.[13] $Mn_{0.9}Cr_{0.1}Au_2$ has a finite spontaneous magnetization in zero external field at $T=240$ K which is below the ordering temperature of 330 K. On the other hand, a finite temperature theory of helimagnetism based on the Heisenberg model as given by Kitano and Nagamiya[23] suggests no qualitative changes of the magnetization processes as compared to $T=0$ K. Moreover, Lyons[24] rigorously proved that in a helical magnet described by the Heisenberg model only order-disorder magnetic phase transitions can occur at finite temperatures. The temperature dependent changes of the wave vector of the helix as well as the stabilization of the FM state should therefore be attributed to a temperature dependence of the exchange coupling between the atomic magnetic moments. At finite temperatures, magnetic disorder causes an additional scattering of the conduction electrons[25] that decreases the magnitude of the exchange coupling and, consequently, affects the helical structure. This thermally induced scattering influences the long-range part of the interactions rather than than those for close neighbors. Since the layers of Mn atoms in $MnAu_2$ bct structure are separated by two layers of Au, the thermally induced scattering can have a significant effect on the relevant interlayer exchange coupling, which is highly probable to the case of the Cr doped alloys. The modeling of this process on an *ab initio* level would be a very interesting and challenging task for future investigations.

In summary we have shown that a classical Heisenberg model with parameters calculated from first principles provides a reasonable description of the low temperature magnetism of $MnAu_2$ and $Mn_{1-x}TM_xAu_2$ alloys. In $Mn_{1-x}Cr_xAu_2$ alloys we propose a scenario for the metamagnetic transition, which, in particular, explains the significant lowering of the high-field magnetization as found in experiment. Performing neutron diffraction experiments on $Mn_{1-x}Cr_xAu_2$ would be highly desirable in order to verify this prediction. The differences in the magnetic behavior of the Fe and the Cr doped alloys are related to the different Mn-Fe and Mn-Cr interatomic exchange interactions and they can only partially be attributed to a renormalization of the Mn-Mn exchange interactions due to chemical substitutions. Since the interplane exchange coupling constants in $MnAu_2$ based structures are mediated by conduction electrons moving through the Au planes, it would also be interesting to chemically substitute the Au sublattice which potentially may lead to a strong reduction of the threshold field, while preserving a GMR effect of sufficient size.

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