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Calculation of the Magnetoresistance of YMn_2Ge_2 and $LaMn_2Ge_2$

J. MILANO[1]) and A.M. LLOIS

Laboratorio TANDAR, Centro Atómico Constituyentes, Comisión Nacional de Energía Atómica, Av. Gral. Paz 1499, 1650 Partido de Gral. San Martín, Argentina

Departamento de Física 'J.J. Giambiagi', Universidad de Buenos Aires, Pabellón I, Ciudad Universitaria, 1429 Buenos Aires, Argentina

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We have calculated the diffusive conductivity and ballistic conductance of the layered compounds YMn_2Ge_2 and $LaMn_2Ge_2$. For YMn_2Ge_2 we obtain a negative band contribution to the giant magnetoresistance. For $LaMn_2Ge_2$ we show that the band contribution can already explain the experimentally observed large positive magnetoresistance if a nearly ferromagnetic structure is considered.

Introduction It is well known that magnetic multilayers show giant magnetoresistance (GMR) in the presence of a magnetic field [1]. The study of this phenomenon, both in artificial and natural multilayers as in granular systems, has been of great interest in the last years.

The $ThCr_2Si_2$ type structure [2] is one of the most frequently observed structures in ternary rare earth compounds. Within this structure the intermetallic compounds of the type RM_2X_2 (R rare earth, M 3d transition metals and X = Si or Ge) have been extensively studied (see Fig. 1). They build natural multilayers and their magnetic properties are very interesting and highly dependent on volume and temperature. In particular, the compounds with M = Mn have received a lot of attention due to the large magnetic moment that the Mn atoms acquire in these systems. These compounds order magnetically near room temperature and show a wide variety of magnetic arrangements, which have been experimentally observed [3 to 6]. The richness in the magnetic behavior is a manifestation of the high sensitivity of the magnetism of Mn to the change in the Mn–Mn distances [4].

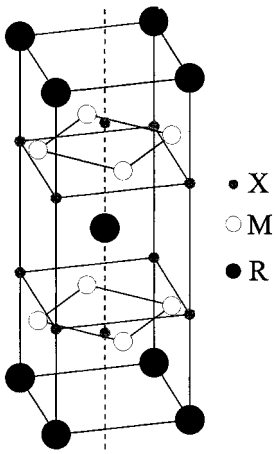

Fig. 1. Crystal structure of the RM_2X_2 compound

[1]) e-mail: milano@cnea.gov.ar

The GMR effect in multilayers is often produced by roughness at the interfaces, which induces an asymmetry in the spin dependent scattering at subsequent interfaces. As these compounds build natural multilayers they have clear cut interfaces and this last contribution to the GMR can be neglected. The GMR for these systems should be, then, mainly due to the electronic band structure.

At low temperatures YMn_2Ge_2 [7] has subsequent in-plane ferromagnetic Mn layers which are antiferromagnetically (AF) coupled along the (001) direction. This system should present the usual direct GMR effect. On the other hand, $LaMn_2Ge_2$ is essentially ferromagnetic (F) [8] and shows experimentally a very large inverse magnetoresistance [9] in the presence of an applied external magnetic field [10]. This inverse GMR has been attributed by some authors to a canting of the Mn magnetic moments [10].

In this work we calculate the electronic and transport properties of $LaMn_2Ge_2$ and YMn_2Ge_2 and obtain the band contribution to the magnetoresistance for both systems by doing ab initio calculations.

Method of Calculation We calculate the ballistic conductance G^i and the conductivity tensor within the semiclassical approximation of conduction. G^i is obtained using the Sharvin model [11] and σ^{ii} is derived from the Boltzmann equation in the relaxation time approximation [12]. The conductivity, which corresponds to the diffusive regime, is then given by

$$\sigma^{ii} = \frac{e^2}{8\pi^2}\,\tau \sum_{\nu s} \int v^i_{\nu s}(\mathbf{k})\, v^i_{\nu s}(\mathbf{k})\, \delta[\varepsilon_{\nu s}(\mathbf{k}) - \varepsilon_{\mathrm{f}}]\, d^3\mathbf{k}\,, \tag{1}$$

where the sum is over the band and spin index ν and s, e is the electron charge, τ the relaxation time, $v^i_{\nu s}$ the semiclassical velocity of the electrons and with i we indicate cartesian coordinates, ε_{f} is the Fermi energy.

The ballistic conductance is given by

$$G^i = \frac{e^2}{h}\, A \sum_{\nu s} \int |v^i_{\nu s}(\mathbf{k})|\, \delta[\varepsilon_{\nu s}(\mathbf{k}) - \varepsilon_f]\, d^3\mathbf{k}\,, \tag{2}$$

where A is the sample cross section perpendicular to the current. In our calculations we take the relaxation time out of the integral and assume that it is independent of the magnetic ordering and of the band index, and obtain the ballistic conductance per unit area [13]. These calculations being within the semiclassical approximation require only the energy bands.

As general expression for the giant magnetoresistance we use

$$\mathrm{GMR} = \frac{G^i(\mathrm{NF})}{G^i(\mathrm{F})} - 1 \quad \text{or} \quad \mathrm{GMR} = \frac{\sigma^{ii}(\mathrm{NF})}{\sigma^{ii}(\mathrm{F})} - 1\,; \qquad -1 < \mathrm{GMR} < +\infty\,. \tag{3}$$

With NF we indicate a non ferromagnetic configuration as, for instance, the AF case or the canted configuration of the Mn magnetic moments in $LaMn_2Ge_2$. The band structure of the systems considered is obtained within the LDA approximation using the Linearized Augmented Plane Wave method (FP-LAPW) as implemented in the WIEN97 code [14] (improved and updated Unix version of the original copyrighted WIEN code, which was published in [15]).

Results and Conclusions With the aim of calculating the band contribution to the GMR we obtain selfconsistently the electronic structure of the systems containing Y

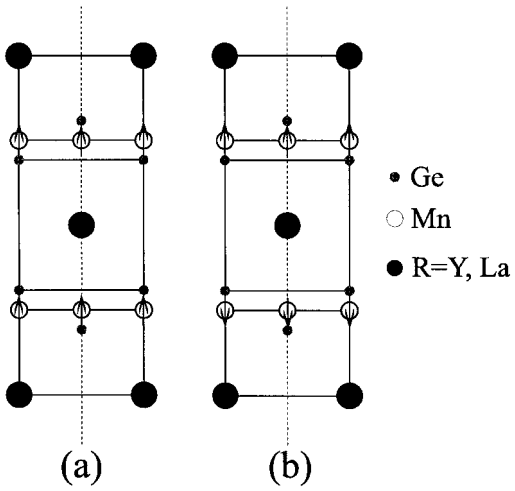

Fig. 2. Schematic view of the a) F and b) AF configurations considered in this work

and La in the F and AF configurations (see Fig. 2). We use in each case the experimental lattice constants [16, 17]. As we know that the ground state of $LaMn_2Ge_2$ is not AF but nearly F (slightly canted), we also simulate this situation constraining the average magnetic moment per Mn atom to be equal to the experimental one by doing a fixed spin moment calculation (FSM) [18]. As the canting of the Mn magnetic moment provides a small in-plane AF contribution, the average magnetic moment is smaller than the one obtained self-consistently for the FM configuration. Namely, in this last configuration the magnetic moment per cell obtained for $LaMn_2Ge_2$ is $8.12\mu_B$ while the experimental value is $6.00\mu_B$.

Selfconsistency in each case is achieved using 1000 k-points in the first Brillouin zone (FBZ). We take for the parameter $R - k_{max}$ a value of 8, this parameter gives the energy cut-off value for the interstitial plane waves [14]. We obtain for the two systems the correct ground state.

For the calculation of conductivity and conductance we use a mesh of 10000 k-points homogeneously distributed in the FBZ. We give in Table 1 the results for the conductivity tensors, the Sharvin conductances and the corresponding magnetoresistances. The units are arbitrary and the values are normalized to the respective transport properties

Table 1

Conductivity (σ), ballistic conductance (G) and giant magnetoresistance (GMR) in the diffusive and ballistic regimes. For $LaMn_2Ge_2$ two possible ground states are considered, the AF and nearly F one (FSM). The values of the conductivity (ballistic conductance) are normalized to the total conductivity (ballistic conductance) of the F state in the z-direction

		YMn_2Ge_2		$LaMn_2Ge_2$		
		F	AF	F	AF	FSM
σ^{zz}		1.00	0.60	1.00	0.65	1.15
σ^{xx}		0.56	0.47	0.57	0.52	0.92
G^z		1.00	0.74	1.00	0.82	1.22
G^x		0.92	0.73	0.89	0.86	1.03
GMR	σ^{zz}		−0.40		−0.35	0.10
	σ^{xx}		−0.16		−0.09	−0.04
	G^z		−0.26		−0.18	0.12
	G^x		−0.21		−0.03	0.15

along the z-direction in the ferromagnetic configuration. In both materials the ballistic conductance is mainly due to the 3d band contribution, while the diffusive conductivity stems from bands of sp character, these last ones are hybridized with 4d bands in the case of the Y containing system and with 5d bands in the other case. As samples of these materials are in general non-nanoscopic, the diffusive conductivities should be the ones considered.

For YMn_2Ge_2 we obtain large negative band contributions to the diffusive magnetoresistance along the z-direction (see Table 1).

For $LaMn_2Ge_2$ we calculate the GMR considering as possible ground states both the AF and the canted (FSM) configurations. In the first case we obtain a negative band contribution to the GMR, while in the other one the band contribution to the GMR can already partly explain the positive GMR experimentally observed, as it is shown in Table 1. This positive contribution stems from a relative shift of majority and minority bands with respect to the AF configuration when the spins are canted. In future work we are going to put the canting explicitly into the Hamiltonian.

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