ELSEVIER

Journal of Magnetism and Magnetic Materials 226–230 (2001) 1755–1757

Journal of magnetism and magnetic materials

www.elsevier.com/locate/jmmm

From direct to inverse GMR: introduction of Cr in Fe/Cu superlattices

J. Milano[a,b,*], A.M. Llois[a,b]

[a]*Lab. TANDAR, CAC, CNEA. Av. Gral. Paz 1499 - (1650) Partido de Gral. San Martín, Argentina*
[b]*Departamento de Física, UBA. Pab. I, Ciudad Universitaria - (1429) Buenos Aires,Argentina*

Abstract

It is well known that layered systems can present giant magnetoresistance (GMR). Particularly, the multilayers $Fe_N/Cu_8/Fe_M/Cr/Fe_M/Cu_8$ show inverse GMR. That is, the electrical conductivity decreases with the applied magnetic field. In the most common multilayers the conductivity increases with the applied field and this kind of GMR is called direct. In general the GMR is attributed to spin-dependent scattering in the bulk and mainly at interfaces. In this work we calculate the electronic band contribution to the GMR for $Fe_3/Cu_4/Fe/Cr/Fe/Cu_4$ and Fe_3/Cu_4 multilayers within the semiclassical approximation. The electrical conductivity is obtained in the ballistic and diffusive regimes. The results show a large change in the GMR behavior when one layer of Cr is introduced within the Fe layers. The GMR calculated in the CPP configuration (current flowing perpendicular to layers) of Fe_3/Cu_4 is of the direct type, with a value of about 40% while that obtained for $Fe_3/Cu_4/Fe/Cr/Fe/Cu_4$ is inverse and of the order of 45%. In the CIP configuration (current flowing parallel to the layers) the calculated GMR is direct with a value of about 35% for the system without Cr while, by the introduction of Cr, we obtain also a direct GMR but of about 3%. © 2001 Published by Elsevier Science B.V.

Keywords: Multilayers—metallic; Magnetoresistance—multilayers; Transport properties; Band structure calculations

With the advent of magnetic multilayers the study of their transport properties has turned into an area of growing interest in the last few years. In particular, giant magnetoresistance effects (GMR) [1] have been observed in a large number of multilayered systems and granular alloys. Most theories try to explain this by spin-dependent scattering at defects either in the bulk or at the interfaces. But actually, band structure effects are also important [2].

GMR can be studied under two different electrical transport regimes: that of diffusive conductivity and of ballistic conductance. Presently available experimental results are obtained in the diffusive limit and are, thus, more adequately interpreted by the diffusive conductivity, σ, than by the ballistic conductance, G. However, the recent production of superlattices, as well as other mesoscopic systems, with mean electronic free paths of the order of magnitude of their thickness has turned the ballistic conductance G into a physical quantity of actual interest.

Two kinds of GMR have been observed: direct and inverse. In the first case the resistivity decreases with the applied magnetic field, while in the second one it increases at least within a certain range of the applied magnetic field strength.

A few years ago, George et al. [3] measured inverse GMR in Fe/Cu multilayers by intercalating thin Cr layers within half of the Fe layers. More recently, inverse GMR has also been reported for the systems $Fe_{1-x}V_x/Au/Co$ and Co/Ru/Co. In all these cases inverse GMR has been attributed to asymmetry in the spin-dependent scattering in adjacent ferromagnetic layers.

On the theoretical side calculations for systems showing inverse GMR have been done within the diffussive

* Correspondence address: Lab. TANDAR, CAC, CNEA. Av. Gral. Paz 1499 - (1650) Partido de Gral. San Martín, Argentina. Fax: +54-11-4754-7121.

E-mail address: milano@cnea.gov.ar (J. Milano).

0304-8853/01/$ - see front matter © 2001 Published by Elsevier Science B.V.
PII: S0304-8853(00)00886-6

regime by the only consideration of impurity scattering effects at interfaces and bulk [4].

The aim of this work is to determine the relative importance of the electronic band contribution to inverse GMR. For this, we consider the multilayered systems Fe_3/Cu_4 (direct GMR) and $Fe_3/Cu_4/Fe/Cr/Fe/Cu_4$, this last system results upon replacement of one Fe layer by a Cr one every two unit cells of the first system. The subindexes indicate the number of atomic layers of the corresponding element. We try to obtain the band changes that take place when moving from one system to the other, which induce the switch from direct to inverse GMR.

The calculations are performed for the electrical current flowing parallel to the layers (CIP geometry) and perpendicular to them (CPP). The experiments have been done in the CIP for the case under study.

The ballistic conductance, G^i, is obtained within the Sharvin model which considers that the electrons move through a zone of smaller dimensions than their mean free path [5]. The conductivity tensor, σ^{ij}, derived from the Boltzmann equation in the relaxation time approximation, and the ballistic conductance are calculated as in Ref. [2]. These atomic calculations require only the energy bands as input.

As general expressions for the giant magnetoresistance we use

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

We indicate ferromagnetic (antiferromagnetic) configuration by F (AF).

The band calculations are done using the WIEN97 code [6]. The local spin density approximation (LSDA) for exchange and correlation as given by Perdew and Wang is used and scalar relativistic effects are included in the calculations.

For the Fe_3/Cu_4 multilayer the magnetic F and AF configurations considered for the calculation of the GMR are schematically given in Fig. 1a and the ones corresponding to the system with Cr appear in Fig. 1b. All interfaces are relaxed to minimize the energy of the systems. We find that Cr has a strong antiferromagnetic coupling with the adjacent Fe layers as observed experimentally. When the magnetic field is applied, the first set of layers to get ferromagnetically aligned are the Fe ones.

Self-consistency in each case is achieved using 167 k-points in the 1st Brillouin Zone (FBZ). We take for the parameter R-Kmax, which gives the energy cut-off value for the interstitial expansion in plane waves, the value of 7 [6].

For the transport calculations we use a mesh of 2800 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.

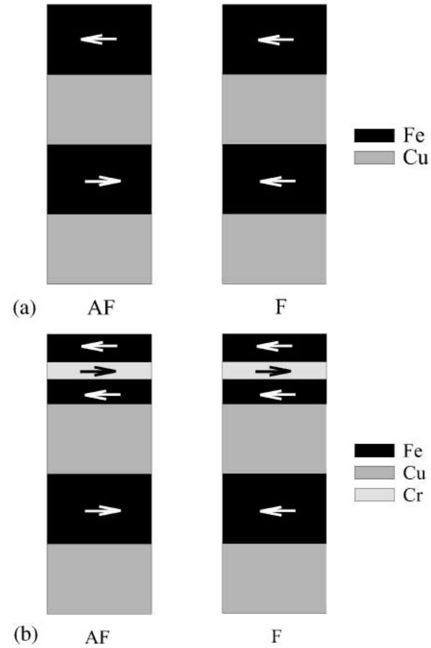

Fig. 1. Schematic view of the F and AF configurations considered in this work. (a) Configurations for the Fe_3/Cu_4 system and (b) for the $Fe_3/Cu_4/Fe/Cr/Fe/Cu_4$ multilayer.

Table 1
Conductivity (σ), ballistic conductance (G) and giant magnetoresistance (GMR) in the diffusive and ballistic regimes. The values of the conductivity (ballistic conductance) are normalized to the total conductivity (ballistic conductance) of the F state of Fe_3/Cu_4 in the x direction

		Fe_3/Cu_4		$Fe_3/Cu_4/Fe/Cr/Fe/Cu_4$	
		F	AF	F	AF
	σ^{xx}	1.00	0.65	0.63	0.61
	σ^{zz}	1.15	0.29	0.22	0.31
	G^x	1.00	0.97	0.91	1.00
	G^z	0.79	0.45	0.33	0.48
GMR	σ^{xx}		−0.35		−0.03
	σ^{zz}		−0.75		0.41
	G^x		−0.03		0.10
	G^z		−0.43		0.46

The introduction of Cr induces a decrease in the values of σ and G for the F configurations. This effect has also to do with a shift of Fermi-level position due to the modification in the number of conduction electrons. These effects are specially pronounced in the CPP geometry. For the system Fe_3/Cu_4 we obtain a negative (direct) GMR in agreement with experiments. The GMR obtained along the z direction is, as expected, higher than the in-plane one.

For $Fe_3/Cu_4/Fe/Cr/Fe/Cu_4$ a big change in the GMR behavior is obtained. The observed GMR values are larger than for the system without Cr and most of them are positive. This means that the band makes an important contribution to the inverse GMR. The experimental values (CIP geometry) for the multilayers with Cr are of the order of 1%, that is inverse but quite small. This is in agreement with the small value we obtain for GMR(σ^{xx}), for which the important outcome is the big change towards an inverse GMR when Cr is introduced.

Acknowledgements

We thank Dr. L. Steren for having brought this problem to our attention. We acknowledge the Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET) and SECyT (grant PICT 03-00105-02043) of Argentina for partial support.

References

[1] M.N. Baibich, J.M. Broto, A. Fert, F. Nguyen Van Dau, F. Petroff, P. Etienne, G. Creuzet, A. Friederich, J. Chazelas, Phys. Rev. Lett. 61 (1988) 2472.

[2] M. Weissmann, A.M. Llois, R. Ramírez, M. Kiwi, Phys. Rev. B 54 (1996) 15335.

[3] J.M. George, L.G. Pereira, A. Barthélémy, F. Petroff, L. Steren, J.L. Duvail, A. Fert, R. Loloee, P. Holody, P.A. Schroeder, Phys. Rev. Lett. 72 (1994) 408.

[4] J. Binder, P. Zahn, I. Mertig, J. Magn. Magn. Mater. 165 (1997) 100.

[5] K.M. Schep, P.J. Kelly, G.E.W. Bauer, Phys. Rev. Lett. 74 (1995) 586.

[6] P. Blaha, K. Schwarz, J. Luitz, WIEN97, Vienna University of Technology, Vienna, 1997. (Improved and updated Unix version of the original copyrighted WIEN-code, which was published by P. Blaha, K. Schwarz, P. Sorantin, S.B. Trickey, Comput. Phys. Commun. 59 (1990) 399.)