Proceedings of the 16th Czech and Slovak Conference on Magnetism, Košice, Slovakia, June 13–17, 2016

The Magnetic Equation of State and Transport Properties in Reduced Dimensions

K. Warda* and L. Wojtczak

Solid State Physics Department, University of Łódź, Pomorska 149/153, PL-90236 Łódź, Poland

Basing our considerations on magnetic equation of state applied to the description of magnetic systems of confined geometry we developed the model of calculations of the electrical resistivity for metallic multilayers. It was shown that in the transport of charge in ferromagnetic material d-electrons play an important role. The key parameters in the presented model are: the width of the electron energy band and the shift of the energy level for two spin orientations as well as the Fermi energy and size of the sample (the thickness of magnetic and nonmagnetic layers and the total number of layers). The presented results of calculations for temperature dependence of magnetoresistance are in qualitative agreement with the available experimental data. The model calculations introduced in this paper can be applied to current-in-plane geometry as well as to current-perpendicular-to-plane geometry. The calculations are valid within the limitations of the resistor network model.

DOI: 10.12693/APhysPolA.131.878

PACS/topics: 64.30.Jk, 64.60.–i, 75.70.Cn, 72.10.Fk

1. Introduction

We develop a magnetic equation of state for the reduced dimensions [1] in order to calculate the resistance and magnetoresistance of thin films and multilayers. The resistance of the single thin metallic layers was calculated lately by Paja and co-workers [2, 3] for the binary and ternary alloys [4, 5]. The transport properties for trilayers and multilayers were considered in [6].

In Ref. [7] it was shown that the origin of the ferromagnetism in Fe comes from the indirect coupling of the predominately localized d-like electrons through a small number of itinerant d-like electrons. The model suggests that about 5% of the $3d$ electrons are in itinerant bands and 95% are in d-bands which are sufficiently narrow to be considered localized. The band calculations of electronic structure [8, 9] and Fermi-surface measurement confirm this picture [10].

The main aim of this paper is to construct a simple model of calculation of magnetoresistance (MR) for the multilayers. In the literature concerning this subject most models usually describe trilayers. However, the multilayer is composed of few or few tens of cells, which constitutes a complex problem for analytical calculations of MR.

2. Description of model and results

For a multilayer comprising magnetic layers separated by nonmagnetic spacers, there are three different resistivities in the superlattice i.e. the resistivity of two different spin orientations in ferromagnetic (FM) material, and resistivity of the non-magnetic (NM) spacer, which is the same for both spin orientations. In order to estimate the magnitude of all of these resistivities, we assume that the conduction electrons have mainly s and p character, and they are predominantly scattered into the d-band. This mechanism is known as the Mott scattering [11–13]. The resistivity of each spin channel is proportional to the density of states (DOS) at the Fermi level in the d-band, which is in agreement with the Anderson model [14].

The magnetoresistance MR is defined as:

$$MR = (R_{\uparrow\downarrow} - R_{\uparrow\uparrow})/R_{\uparrow\uparrow} \tag{1}$$

where $1/R_{\uparrow\uparrow} = (1/R_{\uparrow} + 1/R_{\downarrow})_{\uparrow\uparrow}$ and $1/R_{\uparrow\downarrow} = (1/R_{\uparrow} + 1/R_{\downarrow})_{\uparrow\downarrow}$, while R_σ is the total resistance in the spin channel σ. The conduction electrons which behave as plane waves can mix the channels, therefore they experience an average resistivity, which in the case of two components is given as

$$\bar{\rho} = (d_1\rho_1 + d_2\rho_2)/(d_1 + d_2). \tag{2}$$

d_1 and d_2 are the thicknesses of the layers, and ρ_1, ρ_2 are the corresponding resistivities.

The resistance of bilayer including FM and NM layers can be written as

$$R_{\uparrow} = \rho_{\uparrow} d_{FM} + \rho_{NM} d_{NM}, \tag{3}$$

$$R_{\downarrow} = \rho_{\downarrow} d_{FM} + \rho_{NM} d_{NM} \tag{4}$$

for spin-up (↑) and for spin-down (↓) orientations. It is worth to stress here that simple classical summations of resistances (relations (3) and (4)) are valid only for incoherent transport.

For parallel magnetization of FM layer, the total magnetization of multilayer which is composed of four layer cells is given by

$$R_{\uparrow\uparrow} = N(2R_{\uparrow}R_{\downarrow})/(R_{\uparrow} + R_{\downarrow}), \tag{5}$$

where N is the total number of four-layer cells in a multilayer, while the total resistance is for antiparallel configuration and it equals

$$R_{\uparrow\downarrow} = N(R_{\uparrow} + R_{\downarrow})/2. \tag{6}$$

The magnetoresistance ratio defined by Eq. (1) is given as

$$MR = (R_{\downarrow} - R_{\uparrow})^2 / (4R_{\downarrow}R_{\uparrow}). \tag{7}$$

The mean value of magnetization $\langle m\rangle$ for the inhomoge-

*corresponding author; e-mail: warda@uni.lodz.pl

neous system for a thin solid film with the thickness n of monoatomic layers can be expressed [1] by

$$\langle m\rangle = \langle m\rangle_{3\mathrm{D}} + \tfrac{1}{n}\left(\langle m\rangle_{2\mathrm{D}} - \langle m\rangle_{3\mathrm{D}}\right),$$

where $\langle m\rangle_{2\mathrm{D}}$ and $\langle m\rangle_{3\mathrm{D}}$ represent the mean value of magnetization for homogeneous 2D and 3D systems. The spontaneous magnetization of the Ising two-dimensional model can be calculated exactly [15] and the value of magnetization is given as

$$\langle m\rangle_{2D} = \left[\frac{1+x^2}{\left(1-x^2\right)^2}\left(1-6x^2+x^4\right)^{1/2}\right]^{1/4} \tag{8}$$

where $x = \mathrm{e}^{-2J/T}$ (J and T denote the exchange constant and the temperature, respectively). By analogy, we can write the expression for the spontaneous magnetization for a homogeneous 3D system [16] as

$$\langle m\rangle_{3\mathrm{D}} = \Big[\frac{1+x^2}{\left(1-x^2\right)\left(1-x^6\right)}\left(1-x^2+4x^4-x^6+x^8\right) \times \left(1-x^2-4x^4-x^6+x^8\right)^{\frac{1}{2}}\Big]^{\frac{3}{4}}. \tag{9}$$

It is usually considered that the conductivity in FM materials is governed by s and p electrons. It was shown that in transport of charge in FM materials d-electrons play an important role [7, 17]. It is worth stressing that the scattering asymmetry is larger for strong FM metals. This fact is due to different DOS for spin up and down orientations at the Fermi level.

The free energy in molecular field approximation for FM layer can be given as

$$F\left(M,N,T\right) = -\frac{1}{k_{\mathrm{B}}T}\sum_{k,\sigma}\ln\left(\exp\left(-\frac{1}{k_{\mathrm{B}}T}\left(E_k-E_{F\sigma}\right)\right)\right) -\frac{1}{2}J_{av}\sum_{k}n_\sigma^2 + \sum_{n_\sigma} n_\sigma E_{F\sigma} + \text{coupling}. \tag{10}$$

In the last formula the symbols mean: E_k is the electron energy with wave number k, n_σ is the total number of electrons with spin σ, $E_{F\sigma}$ — the Fermi energy with spin σ ($\uparrow$ or $\downarrow$), J_{av} — an average exchange interaction between the electrons. The term coupling includes the energy density of the interlayer exchange coupling and, assuming only bilinear coupling, it can be given as

$$\text{coupling} = -J\frac{M_1 M_2}{|M_1|\,|M_2|} = J\cos(\alpha_1-\alpha_2), \tag{11}$$

where M_1 and M_2 are the magnetization of the films on both sides of the interlayer while α_1 and α_2 are the angles of magnetization of adjacent magnetic films with respect to chosen directions. Thus $\alpha_1-\alpha_2$ is the angle of magnetization of the films on both sides of the separating layer.

It was shown that the existence of the interlayer exchange coupling is not important for MR effect [18] and thus it will be omitted in further considerations. The value of magnetization M is given by $M = -\mu_{\mathrm{B}}\left(n_\uparrow - n_\downarrow\right)$ where μ_{B} is the Bohr magneton. The equilibrium magnetization for the considered system can determined from minimization of the electronic free energy with respect to magnetization ($\frac{\partial F}{\partial M} = 0$). The conductivity is determined mainly by the electron at the Fermi level. In the spin conserving process the s electrons with spin up and spin down can be scattered to s-band and d-band. The electrons from d-band are exchange split while DOS at the Fermi level is different for spin up and spin down.

The DOS observed experimentally by means of photoemission studies for transition metals exhibits a strong dependence on the surface states [19]. The DOS calculated for Fe using relatively simple method calculations [20] can be useful to predict the magnetic moments which are in agreement with experimental data. Since the DOS for the d-band is exchange split the density of state at the Fermi level is different for spin up and spin down electrons. For the calculations we use the following expressions for DOS:

$$D_\sigma = N\left(E_k \pm \varDelta\right)\left(W - E_k \mp \varDelta\right)\Big/W^3, \tag{12}$$

where W is the width of the electron energy band while $\varDelta$ represents the shift of the energy level for two spin orientations.

Dimensionality reduction on the basis of band theory of magnetism shows that the effect of narrowing bands leads to an increase in the density of states at the Fermi level.

In the model presented in this paper, the density of states at the Fermi level is inversely proportional to the bandwidth.

Finally we obtain the following expression for MR value:

$$MR = \frac{\left(\rho_\uparrow - \rho_\downarrow\right)^2}{4\left(\rho_\uparrow + \frac{\rho_{NM} d_{NM}}{d_M}\right)\left(\rho_\downarrow + \frac{\rho_{NM} d_{NM}}{d_M}\right)}, \tag{13}$$

because the resistivity of each channel according to the Anderson model is proportional to the density of states in the d-band at the Fermi level i.e. $\rho_\sigma \propto N_\sigma\left(E_{\mathrm{F}}\right)$. Taking into account the last relation and the relations (3), (4), (12) we obtain the expression of MR in the following form:

$$MR = \frac{\varDelta^2\left(\frac{2E_{\mathrm{F}}}{W}-1\right)^2}{\left(\left(\frac{E_{\mathrm{F}}}{W}-\frac{\varDelta}{W}\right)-\left(\frac{E_{\mathrm{F}}}{W}+\frac{\varDelta}{W}\right)^2+\rho_{NM}\left(\frac{d_{NM}W^2}{d_M N}\right)\right)} \times \frac{1}{\left(\frac{E_{\mathrm{F}}}{W}+\frac{\varDelta}{W}\right)-\left(\frac{E_{\mathrm{F}}}{W}+\frac{\varDelta}{W}\right)^2+\rho_{NM}\left(\frac{d_{NM}W^2}{d_M N}\right)}. \tag{14}$$

The results of calculations for MR are presented in Fig. 1 as a function of the parameter $\varDelta$ which represents the shift of the energy level for two spin orientations and the parameter W which represents the width of the electron energy band.

The parameter $\varDelta$ represents the spin splitting and is proportional to the mean value of the magnetization for the considered system and the mean value of the exchange interaction between electrons.

In Fig. 2 we present the calculations of MR based on Eq. (14) as function of reduced temperature t =

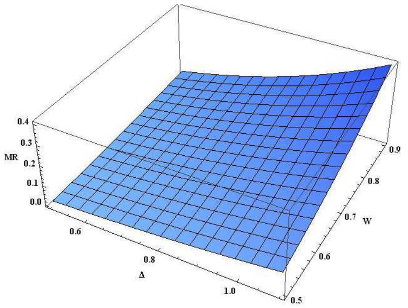

Fig. 1. The MR value as a function of Δ (the shift of the energy level for two spin orientations) and W (the width of the electron energy band) for $d_{FM} = 1.6$ nm and $d_{NM} = 1.2$ nm.

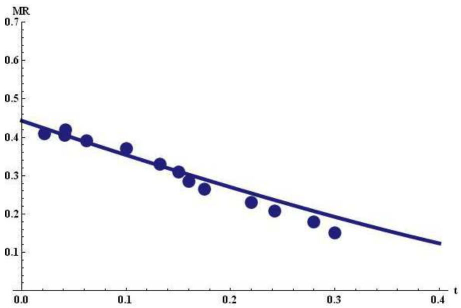

Fig. 2. MR as a function of temperature. The experimental data [21] for Fe/Cr multilayers ($d_{FM} = 1.6$ nm and $d_{NM} = 1.2$ nm, $W = 0.9$ eV) are marked as dots.

T/T_{C}. The obtained numerical results are in qualitative agreement with experimental data [21–23].

3. Conclusions

Using the concept of the equation of state we calculated the transport properties of multilayers. For thin layers the magnetization exhibits the dependence on the number of monolayers in the FM layer. When the number of FM layers increases, the magnetization tends towards the bulk value for the 3D system [1]. The transport properties were examined by means of the equivalent network of resistors for an Fe/Cr/Fe/Cr four layer cells and the equation of state. The model allows to take into account the size effect in the calculations of MR.

The model calculations introduced in this paper can be applied to current-in-plane geometry (CIP) as well as to the current-perpendicular-to-plane (CPP) geometry. The calculations are valid within the limitations of the resistor network model [24, 25].

The main parameters in the introduced model are: the width of the electron energy band, the shift of the energy level for two spin orientations, the Fermi energy as well as the size of the sample (the thickness of magnetic and nonmagnetic layers and the total number of layers). The numerical results show that the temperature behavior of MR is in qualitative agreement with the experimental results [21–23].

References

[1] K. Warda, *J. Phys. Condens. Matter* **21**, 345301 (2009).

[2] A. Paja, A. Działo, *Acta Phys. Pol. A* **125**, 1220 (2014).

[3] A. Paja, A. Działo, *Acta Phys. Pol. A* **123**, 470 (2013).

[4] M. Ornat, A. Paja, *Appl. Phys. A Mater. Sci. Proc.* **102**, 379 (2011).

[5] M. Ornat, A. Paja, *J. Phys. Condens. Matter* **20**, 375102 (2008).

[6] M. Pereiro, D. Baldomir, S.V. Mankovsky, K. Warda, J. Arias, L. Wojtczak, J. Botana, *J. Phys. Condens. Matter* **19**, 106210 (2007).

[7] M.B. Stearns, *Phys. Rev. B* **8**, 4383 (1973).

[8] S. Wakoh, J. Yamashita, *J. Phys. Soc. Jpn.* **21**, 1712 (1966).

[9] K.J. Duff, T.P. Das, *Phys. Rev. B* **3**, 192 (1971); 10.1103/PhysRevB.3.2294*Phys. Rev. B* **3**, 2294 (1971).

[10] A.V. Gold, L. Hodges, P.T. Panousis, D. Stone,- *Int. J. Magn.* **2**, 357 (1971).
brak doi nie znaleziono

[11] N.F. Mott, *Adv. Phys.* **13**, 325 (1964).

[12] G.G. Cabrera, L.M. Falicov, *Phys. Status Solidi B* **61**, 539 (1974); 10.1002/pssb.2220620122 **62**, 217 (1974).

[13] J.M. Ziman, *Electrons and Phonons*, *The International Series of Monographs on Physics*, Eds. N.F. Mott, E.C. Bullard, D.H. Wilkinson, Oxford Univ., London 1960.

[14] P.W. Anderson, *Phys. Rev.* **124**, 41 (1961).

[15] C.N. Yang, *Phys. Rev.* **85**, 808 (1962).

[16] Z.-D. Zhang, *Philos. Mag.* **87**, 5309 (2007).

[17] A. Vedyayev, C. Cowache, N. Ryzhanova, B. Dieny, *J. Phys. Condens. Matter* **5**, 8289 (1993).

[18] J. Barnaś, A. Fuss, R.E. Camley, P. Grünberg, W. Zinn, *Phys. Rev. B* **42**, 8110 (1990).

[19] D.E. Eastman, *J. Appl. Phys.* **40**, 1387 (1969).

[20] W. Zhong, G. Overney, D. Tomanek, *Phys. Rev. B* **47**, 95 (1993).

[21] A. Barthélémy, A. Fert, M.N. Baibich, S. Hadjoudj, E. Petroff, P. Etienne, R. Cabanel, S. Lequien, G. Creuzet, *J. Appl. Phys.* **67**, 5908 (1990).

[22] A. Chaiken, T.M. Tritt, D.J. Gillespie, J.J. Krebs, P. Lubitz, M.Z. Hanrford, G.A. Prinz, *J. Appl. Phys.* **69**, 4798 (1991).

[23] E. Petroff, A. Barthélémy, A. Hamzić, A. Fert, P. Etienne, S. Lequien, G. Creuzet, *J. Magn. Magn. Mater.* **93**, 95 (1991).

[24] D.M. Edwards, J. Mathon, R.B. Muniz, *IEEE Trans. Magn.* **27**, 3548 (1991).

[25] S.F. Lee, W.P. Pratt, Q. Yang, P. Holody, R. Loloee, P.A. Schroeder, J. Bass, *J. Magn. Magn. Mater.* **118**, 1 (1993).