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Surface/interface roughness effects on magneto-electrical properties of thin films

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Abstract

We investigate roughness effects on electrical conductivity and giant magnetoresistance (GMR) in thin films with self-affine roughness, characterized by the r.m.s. roughness amplitude w, the in-plane correlation length ξ, and the roughness exponent H. It is shown that dynamic roughening (evolution of the roughness parameters) plays an important role in electrical conductivity of growing films, and consequently also in the GMR. In both cases our theoretical predictions are in qualitative agreement with experimental observations.

Keywords: Electrical transport (conductivity, resistivity, mobility, etc.); Magnetic films; Surface structure, morphology, roughness, and topography; Magnetic interfaces

1. Introduction

Deviation of thin film surfaces/interfaces from flatness may have a substantial effect on their physical properties, e.g., on magnetic coercive and demagnetizing fields, domain walls, electrical conductivity, giant magnetoresistance (GMR), and others [1–5]. In many cases the surface/interface roughness of deposited thin films is well described in terms of self-affine scaling, which is characterized by the r.m.s. roughness amplitude w, the in-plane correlation length ξ, and the roughness exponent $0 < H < 1$ associated with short wavelength ($<\xi$) roughness irregularity [1,5].

For single-layer thin films, electron scattering by random roughness changes the magnitude and shape of the oscillations due to quantum size effects (QSEs). This, however, depends on the form of the corresponding roughness correlation function associated with the nature of roughness at short (roughness exponent H) and long wavelengths (roughness parameters w and ξ) [2,6–8]. In addition, the film growth mode as well as cross-correlation roughness effects can also strongly influence the electrical conductivity of thin films [7].

Electrical resistance of magnetic multi-layered structures is usually smaller when the magnetic moments of ferromagnetic layers are parallel and larger when they are antiparallel. This difference is known as the GMR effect [9], which can be accounted for by taking into account spin asymmetry of the parameters describing electronic transport in the two spin channels (spin dependent

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scattering probabilities and spin dependent electronic band structure) [10–12]. Generally, GMR is sensitive to the roughness exponent H [17], and also to the cross-correlation between roughness of consecutive interfaces [18]. For magnetic multilayers (i.e., Fe/Au, Co/Cu, Fe/Cr), the roughness exponents in the range $0.3 < H < 1$ have been found experimentally by X-ray scattering measurements [13–15]. Moreover, experimental data show that GMR increases with increasing roughness [14]. This is generally true for small values of the roughness amplitudes, whereas for larger amplitudes the GMR effect decreases with increasing roughness [16].

At any rate of the thin film growth, the surface/interface roughness varies during the growth process and therefore changes the film transport properties. In the following we investigate the effects of surface/interface roughness evolution on the electrical conductivity and GMR of thin metallic single-layer and multi-layer films.

2. Electrical conductivity

In this section, we describe briefly the electrical transport theory for the case of a magnetic trilayer system. Reduction of the description to the case of a non-magnetic single-layer film is straightforward.

We assume the spin-polarized free-electron-like model for electronic structure, with the ferromagnetic conduction band being spin-split due to an effective exchange field. We also neglect spin-flip scattering processes. Accordingly, we consider two ferromagnetic films of thickness d_1 and d_2 which are separated by a non-magnetic metallic spacer of thickness d_0. Let $h_b(\vec{r})$ $(b = 1, 2)$ describe random roughness fluctuations, which are assumed to be single-valued functions of the in-plane vector $\vec{r} = (x, y)$ $(\langle h_b(\vec{r})\rangle = 0)$. For each interface we assume an isotropic autocorrelation function $C_b(r) = \langle h_b(\vec{r})h_b(\vec{0})\rangle$ and a non-zero cross-correlation function $C_{12}(r) = \langle h_1(\vec{r})h_2(\vec{0})\rangle$. For simplicity, we assume that the outer film surfaces are perfectly flat and the whole structure is confined by an infinite potential on both sides.

For a particular magnetization configuration, the global in-plane conductivity g, calculated in the Born approximation, is given by [8]

$$g = \frac{2e^2}{\hbar L}\sum_{\sigma}\sum_{v=1}^{N_\sigma}\sum_{v'=1}^{N_\sigma}(E_F - \varepsilon_{v\sigma}) \times (E_F - \varepsilon_{v'\sigma})\left[C_\sigma^{-1}(E_F)\right]_{vv'}, \quad (1)$$

where the matrix elements $[C_\sigma(E_F)]_{vv'}$ consist of terms $[C_\sigma^b(E_F)]_{vv'}$ and $[C_\sigma^{\mathrm{in}}(E_F)]_{vv'}$, which describe incoherent scattering by bulk defects (impurities) and interfaces, respectively, and also a term $[C_\sigma^{\mathrm{cor}}(E_F)]_{vv'}$ describing coherent scattering by consecutive interfaces due to their cross-correlated roughness

$$C_\sigma(E_F)]_{vv'} = [C_\sigma^b(E_F)]_{vv'} + [C_\sigma^{\mathrm{in}}(E_F)]_{vv'} + [C_\sigma^{\mathrm{cor}}(E_F)]_{vv'}.$$

In Eq. (1) N_σ is the number of two-dimensional occupied subbands for spin $\sigma = (\uparrow, \downarrow)$, $\varepsilon_{v\sigma}$ denote the discrete energy levels due to size quantization, and the matrix elements are taken at the Fermi energy E_F. The explicit forms of the matrices $[C_\sigma^b(E_F)]_{vv'}$ and $[C_\sigma^{\mathrm{in}}(E_F)]_{vv'}$ can be found in Ref. [3], whereas those of $[C_\sigma^{\mathrm{cor}}(E_F)]_{vv'}$ in Ref. [18].

3. Roughness model

For self-affine roughness the Fourier transform $C(q)$ of the height–height roughness correlation function scales as $C(q) \propto q^{-2-2H}$ if $q\xi \gg 1$ and $C(q) \propto$ const. if $q\xi \ll 1$ [1,5]. The roughness exponent H is a measure of the degree of surface irregularity [1,5]. Small values of H characterize more jagged or irregular surfaces at roughness wavelengths shorter than the in-plane correlation length ξ (see Fig. 1). Such a scaling behavior is satisfied by [19],

$$C(q) = (2\pi)w^2\xi^2/\left(1 + aq^2\xi^2\right)^{1+H}, \quad (2)$$

where a is determined by the equation $a = (1/2H)[1 - (1 + aq_c^2\xi^2)^{-H}]$ (with q_c being a cut-off parameter such that $q_c = \pi/a_0$, with a_0 being of the order of the atomic spacing, $a_0 \approx 0.3$ nm). Other roughness models are described in Refs. [1,15,20].

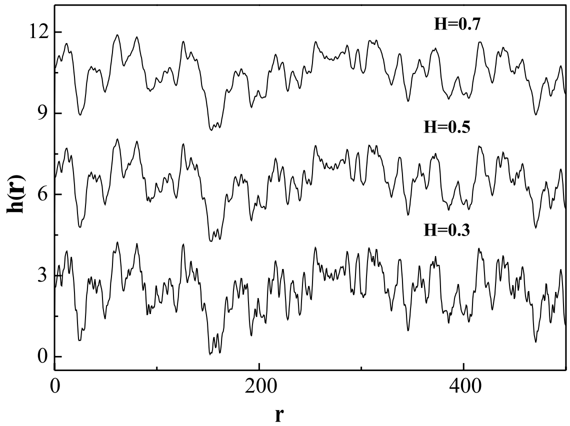

Fig. 1. Roughness profiles with the same roughness parameters w and ξ, but for different values of the roughness exponents H.

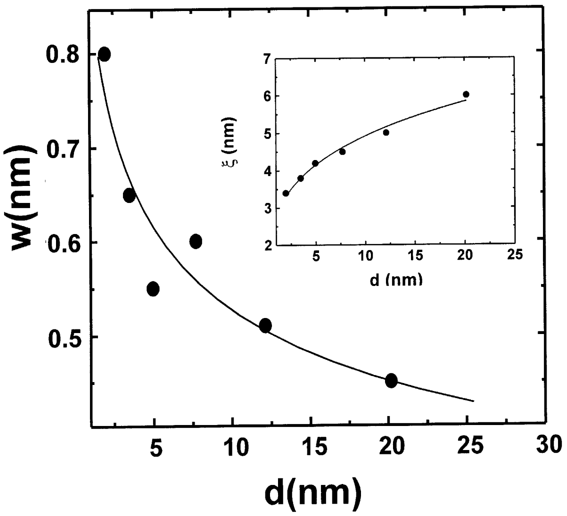

Fig. 2. Evolution of the roughness parameters w and ξ with film thickness as power laws with $w = 14.8d^{-0.22}$ and $\xi = 16.44d^{0.23}$ (in all cases $w < \xi$).

4. Single-layer non-magnetic film

For a single-layer non-magnetic film of thickness d and bulk electron density n, the number of occupied two-dimensional bands N and the Fermi energy E_F can be determined from the condition $nd = (m/\pi\hbar^2)(NE_F - \sum_{v=1,N} \varepsilon_v)$ [2,8].

The roughness correlation function has a significant effect on the conductivity when $\xi q_F > 1$ (with q_F denoting the Fermi wave vector) [2,6,8]. It has been shown theoretically that the transport properties of metallic and semiconducting thin films depend on the roughness exponent H [8]. More specifically, the roughness exponent influences not only size and shape of the QSE oscillations, but also average magnitude of the film conductivity. Apart from this, it has been shown that the conductivity follows the power law $\sigma \propto d^s$, with $s \approx 2.1$–2.3 for small lateral correlation lengths ξ, $\xi q_F \ll 1$ [6]. This power law was successfully used to describe the thickness dependence of the conductivity of $CoSi_2$ films [6]. However, the best fit of the $CoSi_2$ data was obtained for $s = 2.3$ with $w = 0.4$ nm and $\xi = 0.2$ nm ($\xi q_F \sim 1$). Such morphological parameters are quite unphysical because $\xi = 0.2$ nm is smaller than the lattice constant of $CoSi_2$($\sim$0.3 nm) and also $w > \xi$.

The above considerations were based on the assumption that at any thickness the $CoSi_2$ films have the same w and ξ. Our results show that even under the condition of $\xi q_F \gg 1$, one still can obtain an exponent s very close to the experimental results if one includes the dynamic growth effects. Although there is yet no detailed study of the dynamic roughening of solid-phase epitaxy for $CoSi_2$ (since it is a deposition process followed by an annealing process), it is quite reasonable to assume that w will become smaller and ξ larger with increasing film thickness d ($w < \xi$). We assume that both w and ξ are functions of the film thickness d ($w < \xi$ for any thickness). From fitting to the conductivity data we got $w = 14.8d^{-0.22}$ and $\xi = 16.44d^{0.23}$ (see Fig. 2) for $H = 0.5$ and $w < \xi$. Fig. 3 shows the experimental data on electrical conductivity taken from Ref. [6] and our results based on Eq.(1) for $H = 0.5$. At later stages of the growth, the average conductivity increases as a power law with the film thickness, $\sigma \propto d^s$ with $s = 2.4$. Therefore, dynamic roughening process can have a significant influence on the thickness dependence of electrical conductivity.

5. Giant magnetoresistance in multilayers

The GMR effect is described quantitatively by the factor $\mathrm{GMR} = (R_{ap} - R_p)/R_p$, with R_{ap} and R_p

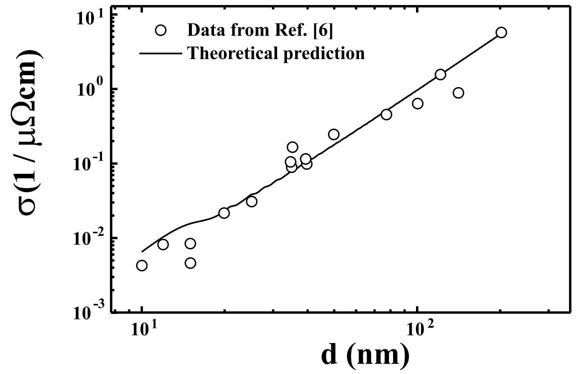

Fig. 3. Conductivity vs. film thickness and theoretical fit for $H = 0.5$ with w and ξ varying as power laws shown in Fig. 2.

denoting the resistances in parallel and antiparallel magnetic configurations, respectively. Our calculations were performed for no bulk scattering ($[C^b]_{\nu\nu'} = 0$), $E_F = 0.3$ eV, $a_0 = 0.3$ nm, $d_1 = d_2 = d_0 = 2$ nm and for symmetrical potential steps at the interfaces; $U_{1+} = U_{2+} = 0.1$ eV for the majority electrons and $U_{1-} = U_{2-} = 0.2$ eV for the minority ones. For simplicity, we assumed the cross-correlated roughness spectrum to be determined by the condition $C_{12}(q) = [C_1(q)C_2(q)]^{1/2}$. The r.m.s. interface roughness amplitudes $w_{1,2}$ were smaller than the sublayer thicknesses, $w_{1,2} \ll d_1, d_2, d_0$.

As follows from Fig. 4, the GMR effect increases monotonically with increasing roughness ratio w_2/ξ_2, or alternatively with increasing interface roughness at constant correlation length or with decreasing correlation length at constant roughness amplitude. This behaviour is in agreement with the GMR data obtained on Fe/Cr multilayers [14]. In fact, upon annealing of the Fe/Cr superlattices, the GMR was found to increase with increasing roughness ratio w/ξ in the temperature range between 20 and 410 °C (see Fig. 7c in Ref. [14] and the inset in Fig. 4). In these experimental studies, the interfaces had almost constant r.m.s. roughness amplitude of $w \approx 0.3$–0.4 nm, and it was found that the lateral correlation length varied during the annealing process (which was assumed the same for all interfaces during the X-ray data analysis [14]). The same situation was assumed in numerical calculations presented in Fig. 4. This case indicates too, that the dynamic evolution of the characteristic roughness parameters has to be taken into account in order to properly describe the GMR data.

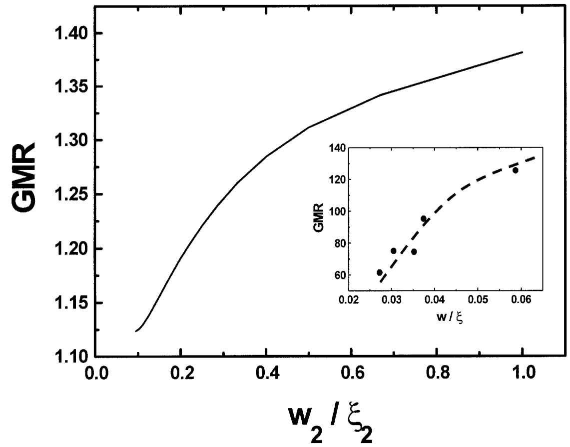

Fig. 4. GMR vs. roughness ratio w_2/ξ_2 for $\xi_1 = 2$ nm, $w_1 = w_2 = 0.4$ nm, and $H_1 = H_2 = 0.8$. The inset shows the data (from Fig. 7c [14]) for qualitative comparison (with the dashed line being a guide for the eye).

6. Conclusions

It has been shown that the interface roughness, as well as its dynamic evolution during the growth process, can strongly influence magneto-electrical transport properties of thin films. Therefore, precise determination of the roughness parameters is necessary for a better understanding, control and performance of microelectronic devices, where the presence of interface roughness is inevitable and can evolve during system growth and/or processing.

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References

[1] Y.-P. Zhao, G.-C. Wang, T.-M. Lu, in: Characterization of amorphous and crystalline rough surfaces-principles and applications, Experimental Methods in the Physical Science, vol. 37, Academic Press, 2000.
[2] G. Palasantzas, Y.-P. Zhao, G.-C. Wang, T.-M. Lu, J. Barnas, J.Th.M. De Hosson, Phys. Rev. B 61 (2000) 11109.
[3] J. Barnas, Y. Bruynseraede, Europhys. Lett. 32 (1995) 167; J. Barnas, Y. Bruynseraede, Phys. Rev. B 53 (1996) 408.
[4] G. Palasantzas, Z.P. Zhao, G.-C. Wang, T.-M. Lu, J.Th.M. De Hosson, Physica B 283 (2000) 199; Z.P. Zhao, G. Palasantzas, R.M. Gamache, G.-C. Wang, T.-M. Lu, J.Th.M. De Hosson, J. Appl. Phys. 89 (2001) 1325.
[5] P. Meakin, Phys. Rep. 235 (1993) 1991; J. Krim, G. Palasantzas, Int. J. Mod. Phys. B 9 (1995) 599.
[6] G. Fishman, D. Calecki, Phys. Rev. Lett. 62 (1989) 1302; G. Fishman, D. Calecki, Phys. Rev. B 43 (1991) 11581.
[7] H. Sakaki, T. Noda, K. Hirakawa, M. Tanaka, T. Matsusue, Appl. Phys. Lett. 51 (1987) 1934; A. Gold, Z. Phys. B 74 (1989) 2100.
[8] G. Palasantzas, J. Barnas, Phys. Rev. B 56 (1997) 7726; G. Palasantzas, J. Barnas, Phys. Status Solidi B 209 (1998) 319.
[9] M.N. Baibich, J.M. Broto, A. Fert, F. Nguyen van dau, F. Petroff, P. Etiene, G. Creuzet, A. Friederich, J. Chazelas, Phys. Rev. Lett. 61 (1988) 2472; G. Binasch, P. Grunberg, F. Saurenbach, W. Zinn, Phys. Rev. B 39 (1989) 4828.
[10] J. Barnas, A. Fuss, R.E. Camley, P. Grunberg, W. Zinn, Phys. Rev. B 42 (1990) 8110; P.M. Levy, S. Zhang, Phys. Rev. Lett. 65 (1993) 1643; R.Q. Hood, L.M. Falicov, D.R. Penn, Phys. Rev. B 49 (1994) 368.
[11] K.M. Schep, P.J. Kelly, G.E.W. Bauer, Phys. Rev. Lett. 74 (1995) 586.
[12] E.E. Fullerton, D.M. Kelly, J. Guimpel, I.K. Shuller, Y. Bruynseraede, Phys. Rev. Lett. 68 (1992) 859; P. Belien, R. Schad, C.D. Potter, G. Verbanck, V.V. Moshchalkov, Y. Bruynseraede, Phys. Rev. B 50 (1994) 9957; J.F. Mackay, C. Teichert, D.E. Savage, M.G. Lagally, Phys. Rev. Lett. 77 (1996) 3925.
[13] R. Paniago, R. Forrest, P.C. Chow, S.C. Moss, S.S. Parkin, D. Cockson, Phys. Rev. 56 (1997) 13442; T. Gu, A.I. Goldman, M. Mao, Phys. Rev. B 56 (1997) 6474.
[14] R. Schad, P. Belien, G. Verbanck, V.V. Moshchalkov, Y. Bruynseraede, H.E. Fisher, S. Lefebvre, M. Bessiere, Phys. Rev. B 59 (1999) 1242.
[15] S.K. Sinha, E.B. Sirota, S. Garoff, H.B. Stanley, Phys. Rev. B 38 (1988) 2297; V. Holy, J. Kubena, I. Ohlidal, K. Lischka, W. Plotz, Phys. Rev. B 47 (1993) 15896.
[16] J. Barnas, Y. Bruynseraede, Thin Solid Films 275 (1996) 148.
[17] J. Barnas, G. Palasantzas, J. Appl. Phys. 82 (1987) 3950.
[18] G. Palasantzas, J. Barnas, J.Th.M. De Hosson, Acta Phys. Pol. A 97 (2000) 495.
[19] G. Palasantzas, Phys. Rev. B 48 (1993) 14472; G. Palasantzas, Phys. Rev. B 49 (1994) 5785.
[20] G. Palasantzas, J. Krim, Phys. Rev. B 48 (1993) 2873; G. Palasantzas, Phys. Rev. E 49 (1994) 1740.