Analytical approach to the Camley-Barnaś theory for giant magnetoresistance in magnetic layered structures

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We present an analytical treatment of the Camley-Barnaś theory of the magnetoresistance (MR) in magnetic layered structures and obtain an exact and general expression for the MR. Particular attention is given to the multilayer effect for the enhancement of MR change. It is proposed that the MR formula obtained from a single sandwich system can be used to calculate the MR effect of a multilayer structure provided an effective specularity factor for the reflection by the surfaces is introduced as a function of the number of bilayers. The theoretical results are in good agreement with experimental data for the epitaxial $(Fe/Cr)_n/Fe$ multilayers.

Reports of giant magnetoresistance (MR) in ferromagnetic multilayers with antiferromagnetic coupling have attracted great interest for fundamental physics as well as for applications. A very large MR effect was first found in Fe/Cr layered structures. A MR as high as 50% was reported for [Fe(30 Å)]/[Cr(9 Å)] superlattices at liquid-helium temperature,[1] while approximately a 1.5% MR effect was observed in a [Fe(120 Å)]/[Cr(10 Å)]/[Fe(120 Å)] sandwich at room temperature.[2] More recently, a similar effect has been observed in other magnetic layered structures composed of a ferromagnetic metal such as Co or Fe alternated with a nonmagnetic metal such as Cu, Ru, Ag, or Au.[3]

The resistance in a magnetic layered structure depends mainly on the relative angle between the magnetizations of two neighboring ferromagnetic films separated by a nonmagnetic film. Experimental results show that the resistance is largest when the magnetizations of the neighboring magnetic films are antiparallel due to an antiferromagnetic coupling between them and smallest when they are brought into parallel alignment by an external magnetic field. Thus, unlike in common metals, the resistance decreases with field strength, from the maximum at zero field to the minimum at saturation field. The MR is defined as the resistance decrease divided by the resistance of the sample at saturation.[4]

Theoretical investigations[4–8] of the giant MR have focused upon the effects of spin-dependent scattering at the interfaces, as well as within the magnetic films. A theoretical model was worked out by Camley and Barnaś.[4] They have extended a semiclassical approach of the Fuchs-Sondheimer type[9] to the magnetic layered systems including the spin-dependent interface scattering and obtained numerical results for the MR which are compatible with experiments. Recently, an attempt has been made by Barthélémy and Fert[6] to obtain analytical results for the MR instead of numerical solutions. However, their approximate derivation is suitable only for two limits where the magnetic film thickness is either much greater or much smaller than the mean free path.

The purpose of the present Brief Report is twofold. Our first goal is to use the semiclassical approach of Camley and Barnaś[4] to derive analytically exact and general expressions for the MR of magnetic layered structures. The other goal is to attempt to account for the multilayer effect for the enhancement of MR change. To our knowledge the understanding of this effect has not yet been satisfactory. We will replace an actual multilayer structure with a specularity factor R at the outer surfaces by an equivalent single sandwich system with an effective specularity factor $R_{\rm eff}$ so that the multilayer effect can be transformed in part into the influence of $R_{\rm eff}$ on the MR. The other factor of the multilayer effect is considered to be the increase of the interface roughness with increasing the number of bilayers. This factor has been observed in recent experiments.[10] By use of a set of reasonable parameters, our calculated results are shown to be in good agreement with the experimental data for epitaxial $(Fe/Cr)_n/Fe$ structures.

Let us consider the case of a sandwich structure, for example, a Fe/Cr/Fe sandwich with Fe films of thickness b and Cr film of thickness $2a$. Its geometry and the coordinate system used in the following theoretical description are shown in Fig. 1. In the Fushs-Sondheimer-type theory, the scattering due to surfaces and interfaces is ex-

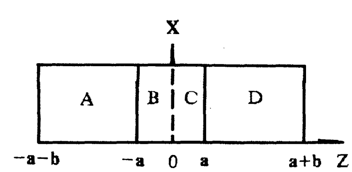

FIG. 1. Geometry of a sandwich structure.

pressed by boundary conditions.[9] For an electric field E along the x direction, the Boltzmann equation has the form

$$\frac{\partial g_s}{\partial z}+\frac{g_s}{\tau v_z}=\frac{eE}{mv_z}\frac{\partial f_0}{\partial v_x} . \tag{1}$$

Here f_0 is the equilibrium distribution function and $g_s(v,z)$ is the correction to the distribution function. The general solution of Eq. (1) is of the form

$$g_s(v,z)=\frac{eE\tau}{m}\frac{\partial f_0}{\partial v_x}\left[1-X_s^{\pm}(v_z)\exp\left[\frac{\mp z}{\tau|v_z|}\right]\right] , \tag{2}$$

where the superscript + stands for electrons with $v_z>0$ and − for electrons with $v_z<0$. The space of the sandwich has been divided into four regions: $X=A$ for $-a-b<z<-a$, $X=B$ for $-a<z<0$, $X=C$ for $0<z<a$, and $X=D$ for $a<z<a+b$. $X_s^{\pm}$ is the coefficient for electrons with spin s in region X, moving to the right ($v_z>0$) or left ($v_z<0$). The spin up ($s=\uparrow$) and spin down ($s=\downarrow$) are defined as the majority- and minority-spin directions, respectively.

All the coefficients $X_s^{\pm}$ can be deduced from boundary conditions at the surfaces and the Fe/Cr interfaces of the sandwich.[4] Here we wish to use some symmetry relations to simplify their derivation. From the invariance of Eq. (1) under reversals of both v_z and z ($v_z\to -v_z$ and $z\to -z$), the solution (2) must satisfy the symmetry relation $g_s(v_z,z)=g_s(-v_z,-z)$, which leads to

$$A_s^{\pm}(v_z)=D_s^{\mp}(-v_z) , \quad B_s^{\pm}(v_z)=C_s^{\mp}(-v_z) . \tag{3}$$

The above conditions, together with the symmetry requirement of $X_{\uparrow}^{\mp}(v_z)$ and $X_{\downarrow}^{\mp}(v_z)$, can reduce the amount of work in determining all the coefficients by a factor of 4.

The plane $z=0$ is not a true boundary; it is the position at which there may be a change in the axis of quantization for the electron spin. When the magnetizations of the two Fe films are parallel, there is no change in the quantization axis so that $g_s(v_z,B)=g_s(v_z,C)$ at $z=0$. It then follows from Eq. (3) that

$$B_s^{+}(v_z)=C_s^{+}(v_z)=B_s^{-}(-v_z)=C_s^{-}(-v_z) . \tag{4}$$

For the antiferromagnetic (AF) configuration, the majority-spin direction (spin up) in regions A and B is opposite to that in regions C and D. So when an electron with spin up in region B crosses the plane $z=0$ and enters region C, it will be regarded as spin down due to the reversal of the quantization axis at $z=0$. Thus, in this case, we have $g_s(v_z,B)=g_{-s}(v_z,C)$ at $z=0$, where $-s$ denotes the spin antiparallel to s. It then follows from Eq. (3) that

$$B_s^{+}(v_z)=C_{-s}^{+}(v_z)=B_{-s}^{-}(-v_z)=C_s^{-}(-v_z) . \tag{5}$$

Taking conditions (3)–(5) into account, one finds that there are only six unknown coefficients; A_s^{+}, A_s^{-}, and B_s^{+} with $s=\uparrow$ and $\downarrow$. They can be determined through the boundary conditions given in Ref. 4 where a spin-dependent transmission parameter T_s ($s=\uparrow$ or $\downarrow$) at the Fe/Cr interfaces has been introduced. With the aid of the solutions for A_s^{+}, A_s^{-}, and B_s^{+} with $s=\uparrow$ and $\downarrow$, we can proceed with the calculation for the conductivity σ(F) of the ferromagnetic configuration and σ(AF) of the AF configuration. The average current density of a sandwich system is given by

$$J=\left[\frac{-em^3}{2(a+b)h^3}\right]\sum_s\int v_x g_s(v,z)d^3v\,dz . \tag{6}$$

After a lengthy evaluation process, we arrive at the following expressions for $\sigma(\mathrm{F})=\sigma(\uparrow,\uparrow)+\sigma(\downarrow,\downarrow)$ and $\sigma(\mathrm{AF})=\sigma(\uparrow,\downarrow)+\sigma(\downarrow,\uparrow)$:

$$\frac{\sigma(i,j)}{\sigma_0}=1-\frac{3\lambda}{8(a+b)}[I_{ij}(\mathrm{Fe})+I_{ij}(\mathrm{Cr})] , \tag{7}$$

where $\sigma_0=ne^2\tau/m$ is the conductivity of the bulk metal and

$$I_{ij}(\mathrm{Fe})=\int_0^1 du\,(1-u^2)u\,(1-E_b)\frac{(1-T_i)(1+T_jE_a^2)(1+RE_b)+(1-R)(1+T_iT_jE_a^2E_b)}{1-T_iT_jRE_a^2E_b^2} , \tag{8}$$

$$I_{ij}(\mathrm{Cr})=\int_0^1 du\,(1-u^2)u\,(1-E_a^2)\frac{(1-T_i)(1+T_iRE_b^2)\gamma_{ij}+(1-R)T_iE_b}{1-T_iT_jRE_a^2E_b^2} . \tag{9}$$

Here $E_a=\exp(-a/\lambda u)$ and $E_b=\exp(-b/\lambda u)$, with λ the mean free path, and

$$\gamma_{ij}=(1+T_j^2RE_a^2E_b^2)/(1+T_iT_jRE_a^2E_b^2) . \tag{10}$$

Finally, combining Eqs. (7)–(10), we can obtain the MR amplitude defined as

$$(\rho_{\uparrow\downarrow}-\rho_{\uparrow\uparrow})/\rho_{\uparrow\uparrow}=[\sigma(\mathrm{F})-\sigma(\mathrm{AF})]/\sigma(\mathrm{AF}) ,$$

where $\rho_{\uparrow\downarrow}$ is the maximum resistivity at zero field and $\rho_{\uparrow\uparrow}$ the saturation field resistivity.

The analytical expressions (7)–(10) for the MR are one of the major results of the present Brief Report. These general expressions are suitable not only for the two limits of $b\gg\lambda$ and $b\ll\lambda$, as has been discussed in Ref. 6, but also for the range $b\sim\lambda$. Furthermore, the specularity parameter R, which varies between 0 and 1, has been included in our results, while only the case of $R=1$ is considered in the analytical approach of Ref. 6.

In the case of $R=0$, since all the terms including the factor R vanish, the analytical result for the MR has a simple form. From Eqs. (7)–(10) we obtain, for $\Delta\sigma=\sigma(\mathrm{F})-\sigma(\mathrm{AF})$,

$$\frac{\Delta\sigma}{\sigma_0}=\frac{3\lambda}{8(a+b)}(T_\uparrow - T_\downarrow)^2\int_0^1 du(1-u^2)u(1-E_b)^2E_a^2 \ . \tag{11}$$

The $\Delta\sigma$ depends on $T_\uparrow$ and $T_\downarrow$ via $(T_\uparrow - T_\downarrow)^2$, while the σ (AF) has a relatively weak dependence of $T_\uparrow$ and $T_\downarrow$. So the MR, $\Delta\sigma/\sigma(\mathrm{AF})$, varies mainly as $(T_\uparrow - T_\downarrow)^2$, especially in the case of $b \gg \lambda$. If introducing two parameters[4]—the diffusive parameter (being a measure of the interface roughness) $D_s = 1 - T_s$ and the asymmetry parameter $N = D_\uparrow / D_\downarrow$—we find that the MR depends mainly on $D_\uparrow^2(1-1/N)^2$. It means that the MR is the greater, the greater the interface roughness and the larger the asymmetry in spin-up and -down scattering, which is in agreement with the numerical results of Ref. 4.

It is convenient to define a function $\Psi(x) = E_3(x) - E_5(x)$, where $E_n(x) = \int_1^\infty dt \exp(-xt)/t^n$, is the exponential function.[11] Taking into account the approximations $\Psi(x) \cong (2/x^2)e^{-x}$ for $x \gg 1$ and

$$\Psi(x) \cong \tfrac{1}{4} - 2x/3 - (x^2/2)\ln(x)$$

for $x \ll 1$, from Eq. (11) we can further obtain two limiting forms of the MR. In the limit $b \gg \lambda$, a simple formula for the MR can be obtained:

$$\frac{\Delta\sigma}{\sigma(\mathrm{AF})}=\frac{3\lambda}{8(a+b)}(T_\uparrow - T_\downarrow)^2\Psi\left[\frac{2a}{\lambda}\right] \ . \tag{12}$$

It is interesting to note that this formula in the condition of $R = 0$ is equivalent to Eq. (31) in Ref. 6, where R is assumed to be unity. Such an equivalence holds only for the limit $b \gg \lambda$. In this limit, since $E_b = \exp(-b/\lambda u)$ is always much smaller than unity within the region of $1 \ge u \ge 0$, all the terms involving the factor E_b in Eqs. (8)–(10) can be neglected. Consequently, the MR effect is easily shown to be independent of the magnitude of R.

In the opposite limit $b \ll \lambda$, Eq. (11) reduces to

$$\frac{\Delta\sigma}{\sigma_0}=\frac{-3\lambda}{16(a+b)}(T_\uparrow - T_\downarrow)^2[L(0)-2L(1)+L(2)] \ , \tag{13}$$

where

$$L(n) = [(2a+nb)/\lambda]^2\ln[(2a+nb)/\lambda] \ .$$

It is easily shown that for nonzero a the MR vanishes as b goes to zero, and for the case of $a = 0$ an approximate expression is given by

$$\frac{\Delta\sigma}{\sigma(\mathrm{AF})}=\frac{(T_\uparrow - T_\downarrow)^2}{2[T_\uparrow T_\downarrow + \ln(\lambda/b)/\ln(\lambda/4b)]} \ , \tag{14}$$

which increases slowly with λ/b and reaches the maximum $0.5(T_\uparrow - T_\downarrow)^2/(1+T_\uparrow T_\downarrow)$ as λ goes to infinity. Tešanović, Jarić, and Maekawa[12] have pointed out that a semiclassical approach to the conductivity of a film of thickness b is inadequate for very thin, high-purity sample, because when λ/b goes to infinity the conductivity σ diverges as $\ln(\lambda/b)$, yielding a nonphysical result. In the present approach to $\sigma(\mathrm{F})$ and $\sigma(\mathrm{AF})$ of a single sandwich, the same problem exists when $b \ll \lambda$ and $a = 0$, both of them varying as $\ln(\lambda/b)$. However, owing to the cancelation of the factor $\ln(\lambda/b)$ included in $\sigma(\mathrm{F})$ and $\sigma(\mathrm{AF})$, the $\sigma(\mathrm{F})/\sigma(\mathrm{AF})$ ratio seems to be relatively reasonable. Its reliability remains to be determined as compared with that obtained in quantum models.

The conductivities $\sigma(\mathrm{F})$ and $\sigma(\mathrm{AF})$ for a magnetic superlattice system ought not to have any divergent problem. Equation (34) in Ref. 6, including a divergent factor $\ln(\lambda/b)$, does not seem to correctly describe their behavior in the limit $b \ll \lambda$. In the present results for finite R given in (7)–(10), there is no divergent difficulty in $\sigma(\mathrm{F})$ and $\sigma(\mathrm{AF})$. In the limit $b \ll \lambda$, the factor $\exp(-b/\lambda u)$ does not vanish for nonzero u, and so the denominators in Eqs. (8)–(10) cannot be approximated to unity except in the case of $R = 0$. In view of the discussion above, Eqs. (34) and (35) in Ref. 6 look like being more suitable to a single sandwich with $R = 0$ rather than a superlattice system with $R = 1$.

When the condition $b \gg \lambda$ is not satisfied, the MR is sensitive to the value of R. In Fig. 2 we explore the behavior of the MR effect as a function of R for several values of b and $2a$. It is found that the MR always increases with an increasing value of R, and its growth rate depends mainly on the thickness of the Fe films and is insensitive to that of the Cr film. This behavior can be roughly understood as follows. The MR is essentially regarded as the spin-dependent scattering divided by the total scattering. Since the surface scattering is assumed to be independent of spin, its decrease (or the increase of R) will reduce the total scattering, but does not change the spin-dependent scattering portion. Thus a larger value of R always leads to a higher MR.

We now turn our attention to the multilayer effect. Recently Barnaś *et al.*[5] have reported the enhancement of MR change with an increasing number of bilayers in the epitaxial $(\mathrm{Fe/Cr})_n/\mathrm{Fe}$ multilayers. They also attempted there to account for the multilayer effect by using an extended Camley-Barnaś model. A plausible agreement between numerical results and experimental data has been obtained.[5] However, numerical work with excessive parameters may make its physical picture unclear.

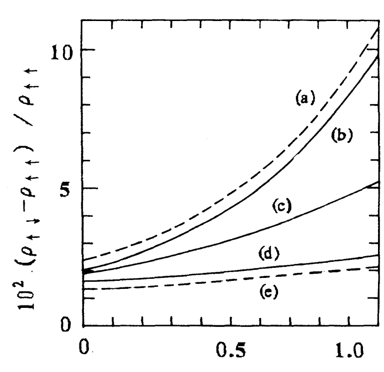

FIG. 2. Variation of the MR as a function of R for several thicknesses of the Fe and Cr films: (a) $2a = 6$ Å and $b = 30$ Å, (b) $2a = 10$ Å and $b = 30$ Å, (c) $2a = 10$ Å and $b = 60$ Å, (d) $2a = 10$ Å and $b = 120$ Å, and (e) $2a = 20$ Å and $b = 120$ Å. The other parameters assumed here are $D_\uparrow = 0.48$, $N = 6$, and $\lambda = 200$ Å.

We wish to interpret the multilayer effect by considering two main factors. The first one is that the interface roughness of multilayer structures increases with an increasing number of bilayers, causing the enhancement of the giant MR effect. Very recently, Fullerton *et al.*[10] have observed the dependences of the x-ray spectra and MR on the number of bilayers. They found that, with increasing n, the Bragg peaks of the multilayer structure broaden and their intensity decreases, indicating that the multilayer roughness increases cumulatively with increasing n. As discussed above, an increasing interface roughness always leads to the increase of the MR effect. Another factor of the multilayer effect is the decrease of the effective surface scattering or the increase of the effective specularity parameter. To understand this point, we note that, with increasing number of bilayers with fixed thickness, both the spin-dependent interface scattering and the nonmagnetic bulk scattering increase in proportion, but the surface scattering remains unchanged, so that the proportion of the surface scattering in the nonmagnetic scattering as a whole becomes smaller and smaller. Thus, if using a single sandwich system to replace equivalently a multilayer structure with n bilayers, we must assume an effective specularity parameter R_{eff} which increases with an increasing n. Such an equivalence enables us to calculate analytically the MR effect of a multilayer structure by using the simple formulas (7)–(10) for a single sandwich system as long as an increasing effective R_{eff} with n is taken into account.

Based on the above argument, we now proceed to fit the present theoretical model to the experimental data. The temperature dependence of the MR observed in the epitaxial $(\text{Fe/Cr})_n/\text{Fe}$ structures with $n=1$, 2, and 4 has been adapted to the mean-free-path λ scale and transformed into MR-vs-λ behavior.[5] These experimental points are shown in Fig. 3, where triangles are for $n=1$, circles for $n=2$, and squares for $n=4$. In order to compare them with our theoretical results, we have used the following parameters in the calculations of Eqs. (7)–(10). The structure parameters are taken to be $2a=10$ Å and $b=100$ Å,[5] and the spin asymmetry parameter of the interface diffusive scattering is assumed to be $N=6$, a value obtained from measurement of the Fe sample with the Cr impurity.[4] The parameters $D_\uparrow$ and R_{eff} are allowed to be different for different samples.

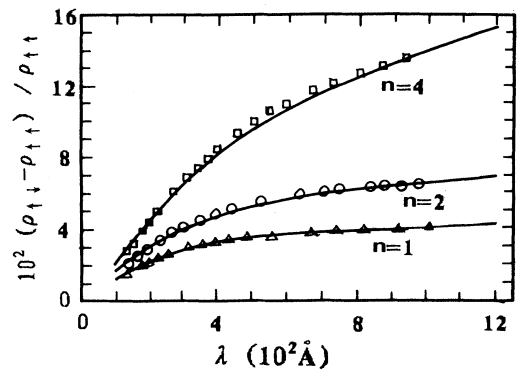

FIG. 3. Theoretical (lines) and experimental (points) magnetoresistivity in the epitaxial $(\text{Fe/Cr})_n/\text{Fe}$ multilayers.

Their values at which the best fit is obtained are $D_\uparrow=0.56$ and $R_{\text{eff}}=0$ for $n=1$, $D_\uparrow=0.62$ and $R_{\text{eff}}=0.2$ for $n=2$, and $D_\uparrow=0.70$ and $R_{\text{eff}}=0.6$ for $n=4$. These values for both $D_\uparrow$ and R_{eff} increase with increasing the number of bilayers, which is quite reasonable as discussed above. With these parameters, our calculated results presented in Fig. 3 (solid lines) give good agreement with the experimental points observed in the $(\text{Fe/Cr})_n/\text{Fe}$ multilayers.

In summary, we have derived an analytical expression for the MR of magnetic layered structures in terms of the semiclassical approach of the Camley-Barnaś model. This result is shown to be suitable to a wide range of b/λ and to all possible values of R. We have further attributed the multilayer effect to an increase in both the effective R_{eff} and the interface roughness with increasing the number of bilayers of multilayer structures. Our theoretical results are shown to be in good agreement with the experimental data observed in the epitaxial Fe/Cr multilayers.

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