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Charge accumulation due to spin transport in magnetic multilayers

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1. Introduction

There is persistent interest in spin transport through magnetic multilayers composed of ferromagnetic (FM) and nonmagnetic (NM) metals due to its importance in physics and promising applications in spintronic devices. Among various configurations, the one with current flowing perpendicularly to the layer plane (CPP) is of particular importance, because it has given rise to many important discoveries and phenomena, such as CPP giant magnetoresistance (GMR) [1] and tunneling magnetoresistance [2].

Spin transport in CPP configuration is characterized by the presence of spin accumulation on the scale of spin diffusion length around the FM/NM interfaces [3]. Valet-Fert theory [4] and other related theories [5,6] show that spin accumulation gives rise to an extra potential drop proportional to a large resistance in FM layers, which is essential to the CPP-GMR effect. It is well-known that electric potential drop is caused by charge accumulation according to Poisson's equation and thus the spin accumulation should coexist with certain charge accumulation in the FM layers. However, the charge accumulation was not calculated in these theories. This inadequacy is our first motivation to study the charge accumulation in detail. Recently, theoretical works [7-9] have shown the connection between the spin and the charge accumulation by different methods. Ref. [9] also predicts that this charge accumulation causes a shortening of the spin diffusion length in FM metals. Unfortunately, the charge accumulation was not

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ABSTRACT

Starting with the Valet–Fert theory of the current-perpendicular-to-plane giant magnetoresistance, we studied the charge accumulation due to spin transport in magnetic multilayers by solving Poisson's equation analytically. Our results show that, in ferromagnetic layers, the charge accumulation has two exponential terms with opposite signs and different decaying lengths: the Thomas–Fermi screening length (on the order of angstrom) and the spin diffusion length (tens of nm in 3d ferromagnetic metals). The charge accumulation on the scale of the screening length is spin-unpolarized and also present in spin-independent transport in nonmagnetic multilayers. However, the charge accumulation on the scale of the spin diffusion length is spin-polarized and shows up only in ferromagnetic layers. Our analysis also provides new insights into the widely used quasi-neutrality approximation, which neglects the charge accumulation.

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calculated in an explicit way and its characteristics were not discussed in depth either. Moreover, charge accumulation is crucial to the magnetocapacitance of magnetic multilayers, which is an important effect besides the GMR effect in CPP configurations [10–12]. There are still controversies over magnetocapacitance effect from both theoretical and experimental aspects [13–15]. Finally, it is also worthwhile to reexamine the widely used quasineutrality approximation, which neglects the charge accumulation. In view of the reasons above, it is necessary to give a detailed analysis on the charge accumulation in CPP magnetic multilayers.

We derived the equations of the charge accumulation by solving Poisson's equation on the basis of the Valet–Fert theory, which is developed by starting with the Boltzmann equation and justified by various experiments. This theory has been extended to include time-dependence [16] and thus our equations for the charge accumulation can also be generalized easily in a similar way.

This paper is organized as follows. In Section 2, we derive the equations of the charge accumulation starting from the Valet–Fert theory. Then we apply these equations to a FM/NM junction in Section 3 and discuss the results in Section 4. The main conclusions and outlooks are given in Section 5.

2. Basic theory

In this section, we will extend the Valet–Fert theory [4] to give the equations of the charge accumulation. The assumptions and notations of Ref. [4] will be kept throughout our derivations and thus some of their results can be used directly. For clarity, we will





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carry out the derivation in the FM layer only, because the corresponding equations of the NM layer can be derived by setting the bulk spin asymmetry coefficient β to be zero and replacing all the parameters of the FM layer by those of the NM layer. Poisson's equation is one-dimensional in this case and can be written as

$$\frac{d^2}{dz^2}V(z) = -\frac{\rho(z)}{\epsilon_0} \tag{1}$$

where V(z) is the electric potential, $\rho(z)$ the excess charge density (that is, the charge accumulation), and ϵ_0 the vacuum permittivity. The charge accumulation $\rho(z)$ can be written as (Eq. (20) of Ref. [16] in time-independent case)

$$\rho(z) = n(z) - 2n_s^0 = -eN_s[2\mu(z) - 2\mu^0]$$
⁽²⁾

where n(z) and $2n_s^0$ are the total charge densities at nonequilibrium and equilibrium states, respectively. Here, $\mu(z) = [\mu_+(z) + \mu_-(z)]/2$ is the average chemical potential, μ^0 the chemical potential at equilibrium state, and -e the charge of an electron. Moreover, N_s is the density of states at Fermi level for spin s and we have the identity, $N_+ = N_-$. Substituting the electrochemical potential, $\overline{\mu}_s(z) = \mu_s(z) - eV(z)$, for the chemical potential in Eq. (2), we have

$$\rho(z) = -eN_s[\overline{\mu}_+(z) + \overline{\mu}_-(z) + 2eV(z) - 2\mu^0]$$
(3)

where $\overline{\mu}_s(z)$ is given by Eq. (C1) of Ref. [4]. Substituting Eq. (3) into Eq. (1), we get a screened Poisson equation

$$\frac{d^2}{dz^2}V(z) - \frac{1}{\lambda_{\rm TF}^2}V(z) = g(z) \tag{4}$$

where

$$\lambda_{\rm TF} = \sqrt{\frac{\epsilon_0}{2e^2 N_{\rm s}}} \tag{5}$$

is the Thomas–Fermi screening length (0.55 Å for copper) in threedimensional systems and the nonhomogeneous term g(z) can be written as

$$g(z) = \frac{eN_s}{\epsilon_0} [\overline{\mu}_+(z) + \overline{\mu}_-(z) - 2\mu^0].$$
(6)

Substituting the expressions of $\mu_s(z)$ into Eq. (6), we have in the FM layers with "up" magnetization

$$g(z) = \frac{1}{e\lambda_{\text{TF}}^2} \left\{ K_1^{(n)} - \mu^0 + (1 - \beta^2) e\rho_{\text{F}}^* J z. + \beta \left[K_2^{(n)} \exp\left(\frac{z}{l_{\text{Sf}}^{\text{F}}}\right) + K_3^{(n)} \exp\left(-\frac{z}{l_{\text{Sf}}^{\text{F}}}\right) \right] \right\}$$
(7)

where I_{sf}^{F} is the spin diffusion length (60 nm for cobalt) of FM layers. In Eq. (7), *J* is the charge current density, ρ_{F}^{*} the bulk resistivity of the FM layers, and β the bulk spin asymmetry coefficient in the FM layers ($\beta = 0$ in NM layers). The constants of integration $K_{i}^{(m)}$ can be determined by boundary conditions.

In the following, Eq. (4) will be solved analytically. The general solution to Eq. (4) can be written as

$$V(z) = V_{\rm h}(z) + V_{\rm p}(z) \tag{8}$$

where $V_p(z)$ is a particular solution to the nonhomogeneous equation (4) and $V_h(z)$ is the solution to the associated homogeneous equation:

$$\frac{d^2}{dz^2}V(z) - \frac{1}{\lambda_{\rm TF}^2}V(z) = 0.$$
(9)

Solving Eq. (9), we can write the complementary function $V_h(z)$ as

$$V_{\rm h}(z) = C_1 \, \exp\left(\frac{z}{\lambda_{\rm TF}}\right) + C_2 \, \exp\left(-\frac{z}{\lambda_{\rm TF}}\right),\tag{10}$$

where the constants C_1 and C_2 need to be determined by boundary conditions. Using variation of parameters, we can write the

particular solution $V_p(z)$ as

$$V_{\rm p}(z) = C_3 + C_4 z + C_5 \exp\left(\frac{z}{l_{\rm sf}^{\rm F}}\right) + C_6 \exp\left(-\frac{z}{l_{\rm sf}^{\rm F}}\right) \tag{11}$$

where

$$C_3 = (\mu^0 - K_1^{(n)})/e, \tag{12}$$

$$C_4 = -(1 - \beta^2)\rho_F^* J, \tag{13}$$

$$C_{5} = -\frac{(l_{\rm sf}^{\rm F})^{2}}{(l_{\rm sf}^{\rm F})^{2} - \lambda_{\rm TF}^{2}} \frac{\beta}{e} K_{2}^{(n)}, \tag{14}$$

$$C_{6} = -\frac{(l_{\rm sf}^{\rm F})^{2}}{(l_{\rm sf}^{\rm F})^{2} - \lambda_{\rm TF}^{2}} \frac{\beta}{e} K_{3}^{(n)}.$$
(15)

Up to now, we have derived the general equation of the electric potential, V(z), which is one of the key results of this paper and in turn enables us to give the expressions of the electric field, charge accumulation.

It is straightforward to get the equation of the electric field by using E(z) = -dV(z)/dz:

$$E(z) = -C_4 - \frac{C_1}{\lambda_{\text{TF}}} \exp\left(\frac{z}{\lambda_{\text{TF}}}\right) + \frac{C_2}{\lambda_{\text{TF}}} \exp\left(-\frac{z}{\lambda_{\text{TF}}}\right) - \frac{C_5}{l_{\text{sf}}^F} \exp\left(\frac{z}{l_{\text{sf}}^F}\right) + \frac{C_6}{l_{\text{sf}}^F} \exp\left(-\frac{z}{l_{\text{sf}}^F}\right).$$
(16)

The equation of the charge accumulation, $\rho(z)$, can be derived by using $\rho(z) = \epsilon_0 dE(z)/dz$ or Eq. (1):

$$\rho(z) = -\varepsilon_0 \left[\frac{C_1}{\lambda_{\text{TF}}^2} \exp\left(\frac{z}{\lambda_{\text{TF}}}\right) + \frac{C_2}{\lambda_{\text{TF}}^2} \exp\left(-\frac{z}{\lambda_{\text{TF}}}\right) + \frac{C_5}{(l_{\text{sf}}^5)^2} \exp\left(\frac{z}{l_{\text{sf}}^5}\right) + \frac{C_6}{(l_{\text{sf}}^5)^2} \exp\left(-\frac{z}{l_{\text{sf}}^5}\right) \right].$$
(17)

The spin-up and spin-down components, $\rho_+(z)$ and $\rho_-(z)$, of the charge accumulation $\rho(z)$ can be derived by using Eq. (A12) of Ref. [16]:

$$\rho_{s}(z) = n_{s}(z) - n_{s}^{0} = -eN_{s}[\mu_{s}(z) - \mu^{0}], \qquad (18)$$

where $n_s(z)$ and n_s^0 are nonequilibrium and equilibrium charge densities for spin *s*, respectively. Substituting $\mu_s(z) = \overline{\mu}_s(z) + eV(z)$ into Eq. (18), we have

$$\rho_{\pm}(z) = -\frac{\epsilon_0}{2} \Biggl\{ \frac{C_1}{\lambda_{\text{TF}}^2} \exp\left(\frac{z}{\lambda_{\text{TF}}}\right) + \frac{C_2}{\lambda_{\text{TF}}^2} \exp\left(-\frac{z}{\lambda_{\text{TF}}}\right) \\ + \frac{C_5}{(l_{\text{sf}}^F)^2} \exp\left(\frac{z}{l_{\text{sf}}^F}\right) + \frac{C_6}{(l_{\text{sf}}^F)^2} \exp\left(-\frac{z}{l_{\text{sf}}^F}\right) \\ \pm \left[\frac{K_2^{(n)}}{e\lambda_{\text{TF}}^2} \exp\left(\frac{z}{l_{\text{sf}}^F}\right) + \frac{K_3^{(n)}}{e\lambda_{\text{TF}}^2} \exp\left(-\frac{z}{l_{\text{sf}}^F}\right) \right] \Biggr\}.$$
(19)

Using the expression of the average electrochemical potential, $\overline{\mu}(z) = \mu(z) - eV(z) = [\overline{\mu}_+(z) + \overline{\mu}_-(z)]/2$, we can write the average chemical potential, $\mu(z)$, as

$$\mu(z) = \mu^{0} + e \left[C_{1} \exp\left(\frac{z}{\lambda_{\text{TF}}}\right) + C_{2} \exp\left(-\frac{z}{\lambda_{\text{TF}}}\right) + C_{7} \exp\left(\frac{z}{l_{\text{sf}}^{\text{F}}}\right) + C_{8} \exp\left(-\frac{z}{l_{\text{sf}}^{\text{F}}}\right) \right]$$
(20)

where

$$C_7 = -\frac{\lambda_{\rm TF}^2}{(l_{\rm sf}^{\rm F})^2 - \lambda_{\rm TF}^2} \frac{\beta}{e} K_2^{(n)},\tag{21}$$

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