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Multiscale modeling of spin transport across a diffuse interface

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ABSTRACT

We present multiscale calculations to describe the spin transport behavior of the Co/Cu bilayer structure including the effect of the interface. The multiscale approach introduces the connection between the *ab initio* calculation used to describe the electronic structure of the system and the generalized spin accumulation model employed to describe the spin transport behavior. We have applied our model to atomically smooth and diffuse interfaces. The results demonstrate the huge importance of the use of first principle calculations, not only due to the interfacial coordinates optimization but also the magnetic and electronic properties obtained through the electronic structure. The system including the effect of interface with and without the charge fluctuation are studied. The results indicate that changes of electronic structure at the Co/Cu interface give rise to an interfacial resistance distributed over several atomic planes, similar to the effect of interface diffusion. We argue that even atomically smooth Co/Cu interfaces have properties analogous to a diffuse interface due to the variation of electronic structure at the interface.

1. Introduction

The understanding of spin transport and spin torque is of increasing importance for spintronic device applications since the discovery of giant magnetoresistance (GMR) [1,2] and tunnelling magnetoresistance (TMR) [3,4]. These phenomena have opened a new path for spintronic device design such as magnetic tunnelling junction (MTJ) sensors [5] and magneto-resistive random access memory (MRAM) [6] leading to the development of new generations of computer architecture. In addition, read sensors for conventional magnetic recording rely on transport properties to achieve the desired functionality. Both spin transport and spin torque are phenomena strongly affected by the interface structure and properties which will therefore play a crucial role in determining resistance arising from spin-dependent scattering at the interface [7–11]. From the theoretical point of view, the simulation of a general interface between two different materials is of great complexity. The usual and easiest way to proceed is to have both alloys in contact locating the atoms of one of the materials *top*, *hollow*, *bridge* of the other. A more general situation would be when the atoms of both materials are allowed to move across to the interface leading to interdiffusion within the interfacial region. This diffusion leads in a different degrees of roughness depending on how much the alloys have mixed. Roughness at interfaces as well as the interfacial and intralayer scattering is of huge importance in relation to the objective of achieving high magnetoresistance (MR) [12,11,9].

The calculation of resistance and spin transport behavior across the diffuse interface can be investigated by injecting spin current into the magnetic system which subsequently gives rise to the spin accumulation (SA) close to the interface region. Various theoretical models have been proposed to describe the effect of interfacial roughness on the magnetoresistance [13–15], indicating that the nature of interfaces is an increasingly significant factor in the spin torque phenomenon. Theoretical approaches to spin torque are often based on the SA model of Zhang, Levy and Fert (ZLF) [16]. The ZLF theory is essentially a drift-diffusion model which only applies to incoherent systems much larger than the mean free path. However, it is important to note that macroscopic models of the effects of a spin-polarized current are based [17] on the simple addition of spin-torque terms in the Landau-Lifshitz-Gilbert equation and, as shown by Claudio-Gonzalez et al. [18] and Chureemart et al. [19], the phenomenological constants representing the strength of the adiabatic and non-adiabatic terms are not spatially invariant; self-consistent solution of the spin accumulation

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and the magnetization is physically a better choice, and an advanced numerical implementation for micromagnetics has been recently presented by Abert et al. [20]. The proper treatment of interface effects was considered by Brataas et al. [21] who introduced the concept of spin mixing conductance. Here we consider a further important effect of the nature of the interface, firstly related to the electronic properties and secondly to the presence of interfacial roughness; practically inevitable in sputtered devices.

The ZLF model has recently been generalized to allow the investigation of diffuse interfaces [22]. The magnetic ion concentration at any given position of the system, determined via Fick's law, gives rise to a spatial variation of the transport parameters within the interface. The model described in Ref. [22] is based on an approach which allows treatment of systems with spatially varying magnetization structures by calculating the SA in a rotated coordinate system based on the direction of the local magnetization [19]. A feature of the model given in Ref. [19] is the calculation of the SA via the local spin polarization $\mathbf{m}$, equal to the local value of $(n^{\uparrow} - n^{\downarrow})$ where the $n^{\uparrow(\downarrow)}$ represents the density of states (DOS) at the Fermi level, E_F, as follows

$$\frac{d\mathbf{m}}{dt} + (J/\hbar)\mathbf{m} \times \mathbf{M} = -\frac{\mathbf{m} - \mathbf{m}_{\infty}}{\tau_{sf}} \tag{1}$$

where $\mathbf{M}$ is a unit vector along the local magnetization direction, J is the s–d exchange integral and τ_{sf} is the spin-flip scattering time. Calculation of $\mathbf{m}$ is convenient for the case of a current flowing between materials with different m_{∞} [22]. We note that $m_{\infty} = (n^{\uparrow}_{eq} - n^{\downarrow}_{eq})$, where the n_{eq} is the equilibrium bulk value which can be obtained via *ab initio* calculation. Further, the spin accumulation, denoted here δm, is usually defined as the deviation of the local spin polarization from equilibrium, i.e. $\delta\mathbf{m} = (n^{\uparrow} - n^{\downarrow}) - (n^{\uparrow}_{eq} - n^{\downarrow}_{eq}) = (\mathbf{m} - \mathbf{m}_{\infty})$. We use Eq. (1) because, although an additional dephasing term has been introduced by Petitjean et al. [23], it has been shown that this can be absorbed into the damping term used in Eq. (1). The model derives stationary solutions for $\mathbf{m}$ and subsequently the SA $\delta\mathbf{m}$ under the assumption that changes in the magnetization are much slower than the variation of the SA.

In this work, we focus on interface properties and their effect on the spin accumulation. First, we consider an atomically flat interface between two different materials. By means of Density Functional Theory (DFT) calculations we investigate the interface electronic structure and its effect on the spin accumulation. The interface is constructed as a periodic *bcc* structure (See Fig. 1-A1 and B) without any roughness. This multiscale approach will be applied to Co/Cu interface to investigate the spin transport behavior as well as evaluate the interfacial resistance. Secondly, we investigate the properties of a diffuse interface created by modelling interdiffusion between the layers. Interestingly it is demonstrated that the interface resistance is spread over several atomic planes in both cases, showing that modification of the interface electronic structure has a similar effect to that of a diffuse interface. The paper is structured as follows. We first describe the spin accumulation model including the calculation of m_{∞}. We then proceed to investigate the spin accumulation an atomically smooth interface, firstly under the simple assumption of an abrupt change of material properties at the interface. This contrasts strongly with the accumulation calculated for the realistic case taking into account the spatial dependence of m_{∞} from the DFT calculations. Finally we present calculations of the spin accumulation for a diffuse interface, which shows a delocalization of the interface resistance similar to that arising from the spatial variation of m_{∞}.

2. Model description

2.1. Spin accumulation model

The full understanding of the mechanism behind GMR and TMR becomes important for the development of spin electronic technologies. The interface resistance can be calculated from the spin accumulation and subsequently gives rise to GMR. Consequently, the calculation of SA is required in order to gain insight into the spin transport behavior. Here, the SA is defined as the difference of spin-up and spin-down electron populations available from *ab initio* calculations. This is essential to deal with multiple layers with different equilibrium value of SA. The general solution of spin accumulation is solved from Eq. (1) consisting of longitudinal ($\mathbf{m}_{\parallel}$) and transverse components ($\mathbf{m}_{\perp,2}$ and $\mathbf{m}_{\perp,3}$) [22] following the equations

$$\begin{aligned}
\mathbf{m}_{\parallel}(x) &= [m_{\parallel}(\infty) + [m_{\parallel}(0) - m_{\parallel}(\infty)]e^{-x/\lambda_{sdl}}]\hat{\mathbf{b}}_1 \\
\mathbf{m}_{\perp,2}(x) &= [G_2 e^{-x/l_+} + G_3 e^{-x/l_-}]\hat{\mathbf{b}}_2 \\
\mathbf{m}_{\perp,3}(x) &= [-iG_2 e^{-x/l_+} + iG_3 e^{-x/l_-}]\hat{\mathbf{b}}_3,
\end{aligned} \tag{2}$$

in a rotated basis system whose axes $\hat{\mathbf{b}}_1$, $\hat{\mathbf{b}}_2$ and $\hat{\mathbf{b}}_3$ are parallel ($\hat{\mathbf{b}}_1$) and perpendicular ($\hat{\mathbf{b}}_2$ and $\hat{\mathbf{b}}_3$) to the local magnetization. The coefficients $m_{\parallel}(0), G_2$ and G_3 are calculated by imposing continuity of the spin current at the interface [16] and $1/l_{\mp} = \sqrt{(1/\lambda_{sf}^2) \pm (i/\lambda_J^2)}$. The equilibrium value $m_{\parallel}(\infty)$ is the difference between the spin-up and spin-down density of states (DOS) at the Fermi energy obtained from *ab initio* calculations,

$$m_{\parallel}(\infty) = \frac{[DOS_{\uparrow}(E_F) - DOS_{\downarrow}(E_F)]k_B Te}{V} \tag{3}$$

where k_B is the Boltzmann constant, T is the temperature, e is the electron charge and V is the unit cell volume.

2.2. Ab-initio calculation of interface electronic properties

In principle, a model that describes the most general geometry of Co/Cu interface would be composed of a diffuse interface, i.e., a geometry where the atoms belonging to both alloys are "transferred" – after performing a molecular dynamics (MD) simulation, for example – from one alloy to the other, having semi-infinite materials on both sides composed of hundreds of atoms. Unfortunately, to model interfaces in this fashion is of extreme difficulty using pure *ab initio* MD calculations due to the huge number of atoms that would be involved. One possibility would be the use of classical MD simulations but the information regarding the electronic structure would be lost. The reduction of the system size is then mandatory. In the present work, we study interface effects by the simulation of three different model systems. In case 1, the interface is taken as atomically smooth and the material properties change abruptly at the interface. In case 2 the interface is again taken as atomically smooth but the SA will be calculated using atomic layer resolved values of m_{∞} determined by DFT calculations on systems with relaxed atomic positions. The layers will be patterned by means of the contact of Co and Cu alloys with the same 2D periodicity and repeated periodically out–of–plane (001) as shown in Fig. 1-B2.

Finally, in case 3 we will create a simple model of a diffuse interface by the replacement of one Co atom within the interface plane by one Cu (see Fig. 1-A2). Again, atomic layer-resolved values of m_{∞}, calculated by DFT methods after relaxation, are used for the calculation of the SA. In this case, there is a computational price to pay, in which we require large sizes of the simulation supercells, having more atoms in the simulation. However, we can minimize