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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 stucture 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.

Keywords: spin transport, multiscale model, diffuse 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 magnetoresistive 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, 8, 9, 10, 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, 14, 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

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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 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

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

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 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

$$\mathbf{m}_{\parallel}(x) \quad = \quad [m_{\parallel}(\infty) + [m_{\parallel}(0) - m_{\parallel}(\infty)]e^{-x/\lambda_{sdl}}]\ \hat{\mathbf{b}}_1$$

$$\mathbf{m}_{\perp,2}(x) = [G_2 e^{-x/l_+} + G_3 e^{-x/l_-}]\,\hat{\mathbf{b}}_2$$
$$\mathbf{m}_{\perp,3}(x) = [-iG_2 e^{-x/l_+} + iG_3 e^{-x/l_-}]\,\hat{\mathbf{b}}_3, \qquad (2)$$

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,

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

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 figure 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 figure 1–A2). Again, atomic layer-resolved values of m_∞, calcuated 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

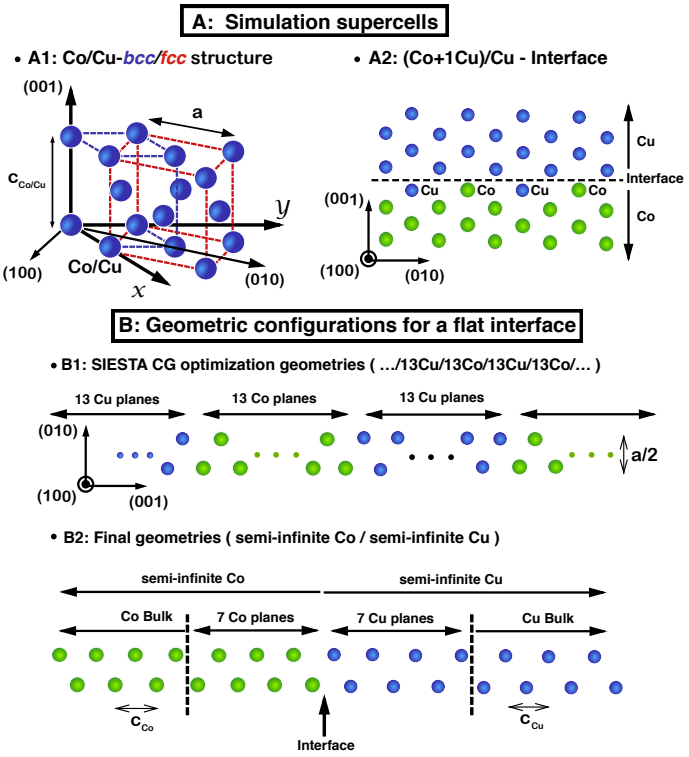

Figure 1: (Color online) (A1) Schematic representation of the Co and Cu *bcc*/*fcc* bulk unit cells; (A2) Side view of the modeled diffusion interface employed in the present work; (B1) Periodic $\cdots$/13Co/13Cu/$\cdots$ geometric configuration used in the conjugate gradient relaxation method; (B2) Final interface geometry between two semi–infinite Co and Cu bulk alloys after extract 7Co+7Cu slice from B1 relaxed coordinates.

the simulation supercells, having more atoms in the simulation. However, we can minimize the computational tasks by choosing conveniently the unit cell. To this end, we observe that in our system the atomic stacking is along the (001) direction and if we inspect the figure 1–A1, we can select either *bcc* or *fcc* to describe the physical systems since both unit cells depict the same structure. The choice of structure will be relevant because of the number of atoms per supercell will be different. Consequently we choose the *bcc* structure due to its reduced number of atoms and because the diffusive interface model will be straightforward to simulate. Subsequently, the spatial magnetic ion concentration is considered from the spatial variation of magnetic moment achieved from the *ab initio* calculations and it is then used to model the spatial diffusive transport parameters. The geometry optimization and the electronic self–consistent (SC) calculations have been performed by means of Density Functional Theory (DFT) using the SIESTA code [24]. As exchange correlation (XC) po-

tential we employed the generalized gradient approximation (GGA) [25]. We used double–ζ polarized (DZP) strictly localized numerical atomic orbitals as basis set. We ensured the convergence of the magnetic moment as well as DOS used in the spin transport calculations by considering 196 k–points.

Fig.1–B describes schematically the construction process of the final $\cdots$Co/Cu$\cdots$ geometry used in this work and its main geometric parameters. Each one of these materials have their own bulk lattice constants and to obtain them we optimized the geometry individually. In doing so the Co and Cu lattice values were 3.54 and 3.68, respectively. We assume that Co and Cu have the same *bcc* structure and that they share the same in–plane lattice constant a, so we chose the mean value to be able to overcome the 4% mismatch between them. On the other hand, in bulk phases a=c, however, when a changes the out–of–plane structure will change and $c_{Co} \neq c_{Cu}$. We performed conjugate gradient relaxation (CG) to determine these out–of–plane parameters ensuring that the final forces between atoms were less than 0.05 eV/. As an initial guess we constructed the configuration shown in 1–B1 for the periodic out–of–plane $\cdots$/13Co/13Cu/13Co/13Cu/$\cdots$ structure. Due to the $\mathcal{Z}$ periodicity no vacuum is needed and each Co/Cu interface experiences the same environment on both sides. This permits to avoid the use of any constraint in the calculation and we were able to select at the end of the optimization 7Co+7Cu planes for the construction of the final geometry 1–B2. In between each two Co/Cu interfaces we ensured with high level of precision that either Co or Cu plane exhibits bulk properties and hence we can join the slab on both sides to the semi–infinite parts. Finally, the resulting out–of–plane values were: c_{Co}/a=0.96, c_{Cu}/a=1.06 and for the common in–plane a, 3.61. For the diffuse interface optimization, the same procedure was followed.

The diffusion of the magnetic ion concentration at any position for the $\cdots$Co/Cu$\cdots$ ferromagnetic/non–magnetic (FM–NM) structure is considered from the spatial variation of magnetic moment achieved from the *ab initio* calculations. The spatial concentration of magnetic ion (Co) at any given position x of the system can be modeled as the following equation,

$$C_{Co}(x) = \frac{N_{Co}(x)\mu_{Co} + N_{Cu}(x)\mu_{Cu}}{[N_{Co}(x) + N_{Cu}(x)]\mu_{Co}} \tag{4}$$

where $N_{Co,Cu}(x)$ is the number of local ion of Co or Cu at any position x and $\mu_{Co,Cu}$ denotes the magnetic moment of Co or Cu. The calculated concentration from Eq. (4) is used to model the spatial variation of the diffusive transport parameters, $P(x)$, taken as a linear combination of the bulk parameters weighted by the local concentrations given by,

$$P(x) = P_{Co}C_{Co}(x) + P_{Cu}[1 - C_{Co}(x)] \tag{5}$$

where $P_{Co,Cu}$ is the diffusive transport parameters of Co or Cu.

3. Results

To describe the physical mechanism of spin transport including the diffuse interface, we study the structure of the bilayer system of Co/Cu by employing the multiscale model, which calculates the SA with $\mathbf{m}_\infty$ determined from layer resolved *ab initio* information. We consider the bilayer system of Co/Cu with three different interfaces as described earlier. Our general solution of SA is then applied to each system discretized into many thin layers to investigate the spin transport behavior and the interfacial resistance at any position in the system. In the following we consider each case in turn before giving an overall interpretation and drawing conclusions.

3.1. Case 1: ideal interface with step change in properties

We first consider the system with an ideal interface by assuming that the concentration of magnetic ion is constant throughout the Co layer. This case further assumes that the transport properties are spatially invariant in the Co and Cu layers. Specifically, we assume that the equilibrium value of SA, $\mathbf{m}_\parallel(\infty)$, varies discontinuously from the bulk value of Co to that of Cu which is zero. The SA is then investigated by using our modified solution in Ref. [22]. The system is discretized into many thin layers in order to calculate and observe the development of SA and spin current by applying the generalized formalism, which propagates the SA solution layer by layer throughout the system.

As expected, the spin accumulation is not changed throughout Co layers with collinear magnetization as clearly shown in Fig. 2 (top). In addition, we focus on the spin transport behavior at the interface between layers. The SA is discontinuous at the interface corresponding to the discontinuity of the spin transport parameters of Co and Cu layers at the interface. We note that $\mathbf{m}$ in the Co layer decays very slowly in the Cu consistent with experiment, due to its large spin diffusion length [26]. The spatial resistance-area product (RA) can be calculated directly from the SA (δm) and spin current (j_m) as follows,

$$RA = \frac{|\Delta\delta m| a^2 k_B T t_F}{j_m e^2} \tag{6}$$

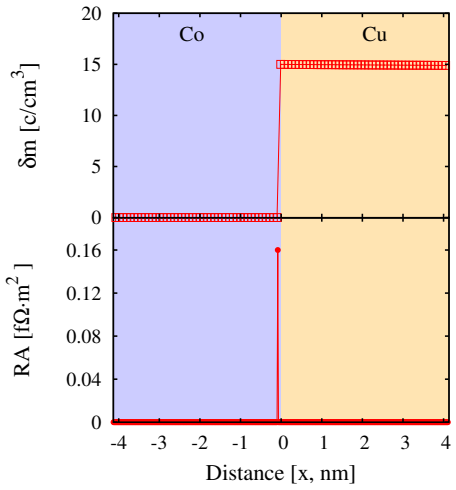

Figure 2: (Color online) (Top) Spatial spin accumulation and (Bottom) Interfacial resistance of the Co/Cu system with an ideal interface, i.e. atomically sharp with a step change of magnetic and transport parameters.

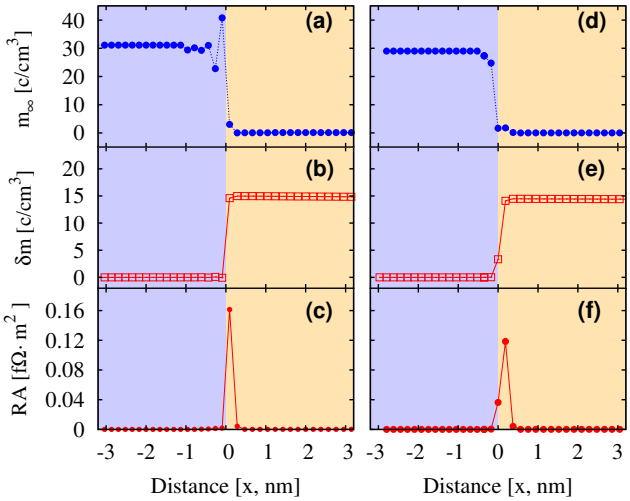

Figure 3: (Color online) (a) (d) Spatial equilibrium value of spin accumulation (b) (e) Spin accumulation and (c) (f) Interfacial resistance of Co/Cu system for Case 2 (sharp interface with ab-initio parameterization) and Case 3 (rough interface) respectively

where $\Delta\delta m$ is the difference of SA across the layers, k_BT is 10 *meV* or 1.6×10^{-21} *J*, a is the lattice constant of material, t_F is the thickness between planes and e is the electron charge. We calculated *RA* between each plane using Eq. (6) as shown in Fig. 2 (bottom). In the Co the corresponding resistance is zero due to the constant value of SA. Similarly in the Cu layer the slow variation of SA leads to essentially zero resistance. The interface resistance is confined to the boundary layer due to the discontinuity in the SA which is consistent with previous study by A. Fert et al. [27]. The total resistance-area product of the structure, a sum of bulk and interface resistances, can be obtained by summing the resistance along the direction of injected spin current. The interface resistance becomes dominant the resistance of the system. The total interface resistance for ideal Co/Cu interface is 0.16 f$\Omega \cdot$m^2 which gives reasonable agreement with both the existing experimental and theoretical values of 0.227 f$\Omega \cdot$m^2 [28, 29, 30].

3.2. *Case 2: atomically sharp interface with* ab initio *parameterization.*

In this case, we study more realistic behavior of spin transport for an atomically structured interface of Co/Cu system by means of the multiscale approach which proceeds by relaxation of the interface and calculation of the DOS. Subsequently it leads to the calculation of the equilibrium value of spin polarization from DOS$_{\downarrow(\uparrow)}$(E$_F$) [22]. The result in Fig. 3 (a) depicts the equilibrium value $\mathbf{m}_{\parallel}(\infty)$ from the *ab initio* calculations. Variations in the DOS close to the interface give rise firstly to a slight polarization of the Cu and secondly to oscillatory behavior in the Co layer close to the interface. The oscillations are due to the interfacial charge rearrangement between both Co and Cu species at the interface. The oscillations in the Co vanish for layers at distances greater than 1 nm, corresponding to the region where the coordinates are similar to those in the Co bulk phase. Using the *ab initio* values of $\mathbf{m}_{\parallel}(\infty)$ we next calculate the SA as a function of position illustrated in Fig. 3 (b). The SA closely follows the equilibrium value since the incoming spin current is fully polarized in the Co layer. Across the interface, the SA exhibits discontinuous behavior due to the different transport properties of the material of Co/Cu, gradually decreasing to zero associated with the spin diffusion length of Cu, (600 nm). Due to the oscillations in the electronic DOS in the Co, one also observes discontinuous behavior of the SA within the Co atomic layers close to the interface with the Cu.

The layer resolved RA is further calculated from SA and the spin current according to Eq. (6) as shown in Fig. 3 (c). The results contrast strongly with that of case 1: the atomically sharp interface with an assumed step change in transport properties, where the interface resistance is fully localized to the interface layer. In Fig. 3 (c) it can be seen that the interface resistance is no longer localized to the Co/Cu boundary. Instead RA is

distributed over several atomic planes around the interface. The phenomenon originates as a result of changes in the electronic structure of Co/Cu close to the boundary. In case 1 we made an implicit assumption that there are no charge fluctuations around the interface region. On the contrary, in the realistic case for Co/Cu interface it is also observable that, even though without species (atoms) transferred between alloys, the properties of a real interface are quite different from those predicted by the simplified model of case 1. The electronic structure modification after the geometry optimization, such as the hybridation between different *s–d* orbitals, indicates that our multiscale model, introducing interfacial effects through the *ab initio* calculations within the atomistic model plays an important role in the prediction of the of the spin transport for any system involving interfaces such as studied here. The interface resistance for this case is 0.172 $f\Omega \cdot m^2$ which is closer to the experimental result [28, 29].

3.3. Case 3: Simple model of a diffuse interface

In practice, sharp interfaces are not expected in real spintronic devices since the sputtering process generally builds diffuse interfaces. As previously mentioned, it is of extreme complexity to perform DFT calculations of these real systems because of the simulation supercell size and hence the large amount of atoms involved. One step forward, compared to the previously studied cases 1 and 2, is the construction of a simple rough interface, where only one atom of one material is replaced by one of the other (see figure 1–A2). In doing so, we take the first step to understand more realistic diffuse interfaces. As in case 2, the rough interface was optimized by means of CG method followed by the self-consistent calculation of the layer resolved DOS. Subsequently $\mathbf{m}_{\parallel}(\infty)$ is determined. In order to compare the present case with previous ones the layer resolved $\mathbf{m}_{\parallel}(\infty)$ values are shown in Fig. 3 (d). It reveals that the polarization extends further into the Cu due to an enhancement of the magnetic moment, and that the rough Co/Cu interface, considerably damps out the oscillations of $\mathbf{m}_{\parallel}(\infty)$ present in the atomically sharp interface. The physical explanation of the reduction in the oscillatory behavior of $\mathbf{m}_{\parallel}(\infty)$ in the present case compared to cases 1 and 2 is lies in the smooth chemical transition between both materials which favors the gradual charge transfer between Co and Cu at the mixed Co/Cu plane.

The transport parameters are estimated from the concentration of magnetic ions. The values of the layer resolved SA is given in Fig. 3(e). We observe that the SA exhibits discontinuous behavior close to the interface and shows damped oscillations compared to case 2. However, the spatial variation of the SA is again delocalized from the interface due to the combination of interface roughness and the spatial dependence on the electronic structure. This is reflected in the layer resolved interface resistance RA as is shown in Fig 3 (f). Similar to case 2 we note that the interface resistance is delocalized from the interface region. For the rough Co/Cu interface, the total RA is approximately 0.175 $f\Omega \cdot m^2$ which is higher than that of ideal interface and consistent with previous studies [28, 29].

4. Conclusions

In conclusion, we employed a recent developed formalism of SA that allows to describe its behavior at any position of any FM–NM interface configuration. In addition, the model makes the possibility for the treatment of systems with sharp variation of SA and also smoothly spatial magnetization concentrations. Furthermore, it is possible to use m_∞ defined as the difference of the $DOS_\downarrow$ and $DOS_\uparrow$ at Fermi level, E_F, quantities readily available from the *ab initio* calculations. Hence, we proposed a multiscale model to give rise the possibility to study the spin transport behavior at any given position of any material through the quantum mechanical calculations and atomistic simulations.

We have applied the multiscale spin accumulation (MSA) model to the Co/Cu interface for 3 cases. Firstly, we considered the ideal case of an atomically smooth interface with a step change in properties at the interface. This system exhibits discontinuous behavior of the spin accumulation and an interface resistance localized to the Co/Cu boundary. We then investigated two more realistic cases, namely, case 2 assuming an atomically smooth interface but with equilibrium polarization calculated from *ab initio* models and case 3 which introduced a first approximation to a rough interface. Both case 2 and case 3 give rise to similar delocalisation of the interface resistance, which is significant over a few lattice spacings. Interestingly, the rough interface gives rise to a smoother variation of the polarization close to the Co/Cu interface. Both case 2 and case 3 exhibit significantly increase values of interface resistance over and above the simplified model of case 1.

Clearly the presence of surface roughness; expected in practice due to the nature of the sputtering process by means of which most systems and devices are produced, has a significant effect on the transport properties as characterized here by the interface resistance. The result of a rough interface is to give rise to an increase of interface resistance which is delocalized from the Co/Cu

boundary and extends over a few lattice spacings. Interestingly, a similar effect is predicted for an atomically smooth interface which might be obtained by MBE. In this case the increased interface resistance and delocalization from the Co/Cu interface results from the modification of the electronic properties of the Co and Cu due to the presence of the interface. The simple model of a bilayer as atomically smooth with a step change in properties is not sufficient, certainly to describe the properties of a Co/Cu bilayer. The properties are determined by a complex mixture of the electronic density of states which gives rise to an oscillatory polarization in the Co and the interface roughness which, although it tends to damp out the DOS oscillations, still results in an increased interface resistance delocalised from the Co/Cu boundary.

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