Experimental separability of channeling giant magnetoresistance in Co/Cu/Co

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The magnitude of the electronic channeling contribution is a significant open issue in the understanding of giant magnetoresistance (GMR). We show that for the technologically important system Co/Cu/Co, channeling GMR can be isolated and quantified experimentally through measurement in the limit of rapid surface diffuse scattering. First-principles based Boltzmann transport calculations are compared with experimental in situ magnetocconductance data, which support the possibility of a significant contribution from channeling. Cyclic control of atomic-scale surface roughness, applied during in situ measurement, will enable a quantitative estimate of the channeling contribution.

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I. INTRODUCTION

Spin-valve giant magnetoresistance, particularly in the technologically important Co/Cu/Co trilayer system, has eluded a complete theoretical description. The relative weights of two separate proposed sources for the current-in-plane giant magnetoresistance (CIP-GMR), spin-dependent diffuse scattering and electronic channeling, could not yet be estimated. In this article, we describe how channeling and spin-dependent scattering contributions to GMR may be separated experimentally in a single Co/Cu/Co “spin-valve” trilayer, allowing quantification as a function of interface microstructures, to which channeling is thought to be especially sensitive.

The most conventional explanation for GMR is given in terms of spin-dependent scattering (SDS). GMR from bulk and interface SDS sum, in the context of the Valet-Fert theory,1 to yield a total \( \Delta R = R_{AP} - R_P \). This additive property, combined with the ability to manipulate bulk SDS alone through selective doping, has enabled experimental separation of bulk and interface SDS contributions to CPP-GMR in the inversion experiments of Hsu et al.2 and Vouille et al.3 Satisfactory agreement between experiments and first-principles-based models of CPP-GMR has been found subsequently.4,5

An additional source of GMR arises in the CIP-geometry due to intrinsic electronic structure and grazing incidence of currents at interfaces. This alternate source, the electronic channeling or “waveguide” effect, has been identified in ab initio calculations of conductivity in the Co/Cu/Co(111) system.6 The channeling contribution to GMR is special since it involves electrons which cannot, at constant \( k_p \), travel from one Co layer to the other. In the parallel magnetization state, spin-up (majority) electrons with large \( k_p \) are confined to the Cu layer since they lack a \( k_p \)-conserving state in majority Co. This reduces the total resistance of the parallel state and is a source of GMR in the absence of spin-dependent diffuse scattering.

The magnitude of the channeling contribution is a major open question in the understanding of GMR. Careful experiments which compare CPP and CIP values for similar structures have simply indicated a “sizable” channeling contribution; Vouille et al.2 attribute the absence of inversion of CIP-GMR to a major role of channeling in CIP.

In this article, we show how the channeling contribution to GMR may be measured and isolated from SDS-related contributions. Using first-principles based Boltzmann transport calculations, we show that the channeling contribution \( \Delta G_{chan} \) is independent of surface scattering, confined as it is to the interior Cu. \( \Delta G_{SDS} \), on the other hand, can be nearly suppressed for high rates of scattering at the exterior Co surface. The two contributions are additive in \( \Delta G \), in analogy to the additive property of bulk and interfacial SDS contributions to \( \Delta R \) measured in CPP. We discuss how in situ magnetocconductance measurement, combined with control over diffuse scattering at the top surface, can be used to separate both contributions in a single sample.

II. MODEL CALCULATIONS

The purpose of the model is to compare any separate size effects of channeling and spin-dependent diffuse scattering GMR in Co/Cu/Co trilayers. The size effect is an important problem in spin valve GMR, as it reduces the GMR of trilayers by nearly an order of magnitude (to 20% at room temperature) compared with multilayer values (to 110%).7,8 Surface diffuse scattering, parameterized by a probability of specular reflection \( p \), is thought to be the origin of this effect. Separate trends in the size effect will motivate an experimental technique to isolate the channeling contribution. We focus therefore on the Co-layer size effect of GMR \( \Delta G(t_{Co}) \) in trilayers and its dependence on the surface specularity parameter \( p \).

A hybrid ab initio/Boltzmann (semiclassical) transport
Figure 1. (Color online) \(k\)-resolved map of contributions to CIP-GMR, measured as \(\Delta G(k) = G_P(k) - G_A(k)\). Left to right: calculations for (100), (110), and (111) oriented Co(20)/Cu(30)/Co(20 Å) trilayers. Top to bottom: perfectly specular top surface scattering \(p_{top} = 1\) to perfectly diffuse top surface scattering \(p_{top} = 0\). The white lines bracket the channeling states in Cu, for which no allowed majority state in Co exists. Note that contributions to \(\Delta G(k)\) are independent of surface scattering. Increasing contributions to \(\Delta G(k)\) represented by ascending brightness in color, from black to yellow.

The model was used to explore the size effects. Effects of band structure are incorporated in two ways. First, *ab initio* LKKR (Ref. 10) derived spin- and \(k\)-dependent interfacial transmission and reflection probabilities are applied to transport across Co/Cu interfaces. Second, spin- and \(k\)-dependent Bloch-wave velocities generate mean-free paths \(\lambda^\ell_s\) from an isotropic spin-dependent relaxation time \(\tau^\ell\). The remainder of the model is fully semiclassical.

The BTE is solved separately for each layer and each energy band intersecting the Fermi surface, at individual values of \(k\), within the first interface Brillouin zone. Total contributions to the current are summed over all layers, bands, and values of \(k\). Calculations were performed for epitaxial trilayers of (100), (110), and (111) orientations. CIP conductances were calculated for in-plane currents in the [001], [110], and [110] directions, respectively.

The focus of the present study is the influence of the surface specularity parameter \(p\). Several other input parameters are necessary in the model, however. Bulk scattering rates are introduced to create resistivities for Cu and Co of 3.8 \(\mu\Omega\) cm and 21 \(\mu\Omega\) cm for Cu and Co, respectively, taken from the experimental *in situ* measured, thickness dependent conductivity \(\sigma(t)\). Large spin asymmetries need to be chosen to reproduce experimental values of GMR; we take the following values from a previous study.\(^9\) A 1:10 ratio for minority: majority lifetimes \(\tau^-/\tau^+\) was chosen in Co to introduce bulk spin-dependent scattering. Spin-dependent interface diffuse scattering is taken into account through the use of a specularity parameter \(S^\ell\neq S^\ell\), with \(1-S^\ell\) giving the fraction of diffuse-scattering events; \(S^\ell\) is taken to be 0.3 and \(S^\ell=1\). Where bulk SDS only is treated, \(S^\ell\) is taken as 1.

Diffuse scattering at bottom and top surfaces, as (bottom): Co/Cu/Co:top, is parameterized using specularities \(p_{top}\) and \(p_{bottom}\). The \(p=1\) condition corresponds to specular reflection and \(p=0\) corresponds to its absence in diffuse scattering. We assumed a specular bottom surface \(p_{bottom}=1\); \(p_{top}\) varies in the calculations.

Calculated values of giant magnetoconductance \(\Delta G\) for Co(20)/Cu(30)/Co(20 Å) trilayers are shown in Fig. 1, resolved to \(k\) points and reduced to the first interface BZ. Results are shown for (100), (110), and (111) oriented trilayers. The heavy white lines indicate regions of electronic channeling in Cu. Between these lines, there are allowed \(k\) states in Cu, but no allowed \(k\) states in the majority fcc Co.\(^{16}\) Electrons which conserve this value of \(k\) are therefore confined to Cu: the transmission probability into Co is zero.

As surface diffuse scattering is increased \((p=1\rightarrow p=0)\), contributions to GMR from lower \(k\) states are suppressed, regardless of crystal orientation. These states, which contribute to GMR through spin-dependent diffuse scattering, are located outside of the regions bounded by white lines in Fig. 1. Spin-dependent reflectivity contributions to GMR, arising as they do from regions where there are allowed states in majority Co, are present in these lower \(k\) states as well. The suppression of SDS-GMR from surface scattering is well known from free-electron models of GMR spin valves.\(^{7,8}\)

Contributions to GMR from states involved in the channeling effect, located at high values of \(k\) corresponding to grazing incidence, remain unchanged. These channeling states are located inside the regions bounded by white lines in Fig. 1. This behavior has not been recognized previously. To the extent that GMR arises from channeling, it is insensitive to surface scattering or the condition of the surface.

As described, SDS- and channeling-related contributions to GMR operate on nonoverlapping sets of \(k\) points, for a given Cu band. In the simulation it is then possible to moni-
tor the contributions of SDS and channeling to GMR, $\Delta G_{\text{SDS}}$ and $\Delta G_{\text{chan}}$ separately. Channeling $k_i$ points are those which lack an allowed state in majority Co, but possess an allowed state in Cu; $\Delta G_{\text{chan}}$ sums over contributions from these points. We have examined the free layer thickness dependence of these independent contributions to GMR.

The size effects of $\Delta G_{\text{chan}}(t_{\text{Co}})$ and $\Delta G_{\text{SDS}}(t_{\text{Co}})$ are shown in Fig. 2. The bottom surfaces are assumed to be fully specular ($p_{\text{bottom}}=1$) in these calculations. The top graph shows $\Delta G_{\text{SDS}}(t_{\text{Co}})$ and $\Delta G_{\text{chan}}(t_{\text{Co}})$ for (111) oriented trilayers, assuming $p_{\text{top}}=0$ and $p_{\text{bottom}}=1$. The middle graph shows the orientational dependence, comparing total and channeling contributions for (100), (110), and (111) trilayers. Finally, the bottom graph compares $\Delta G_{\text{SDS}}(t_{\text{Co}})$ and $\Delta G_{\text{chan}}(t_{\text{Co}})$ for (111) trilayers under assumptions of bulk and combined bulk and interfacial SDS.

It can be seen that channeling and SDS contributions to GMR exhibit entirely different size dependencies in a spin valve. Figure 2 (top, middle) shows that $\Delta G_{\text{chan}}$ is nearly constant as a function of free layer thickness, for all calculated orientations or values of $p_{\text{top}}$. The absence of size effect follows from the independence of channeling contributions to surface scattering, as shown previously in Fig. 1. $\Delta G_{\text{SDS}}$, on the other hand, shows a strong size effect in the case of strong surface scattering ($p_{\text{top}}=0$), and a sizable, exponentially activated difference between the $p_{\text{top}}=0$ and $p_{\text{top}}=1$ conditions. The size effect in $\Delta G$ follows Gurney’s relation \[ \Delta G(t_\ell) \propto 1 - \exp(-t_\ell/\lambda_{\text{SDS}}) \] closely, as derived from free electron models. Extrapolated values of $\Delta G_{\text{SDS}}$ at zero thickness are close to zero for all orientations. This behavior is present irrespective of the location of SDS assumed, as shown in the bottom figure: bulk and interfacial SDS are suppressed in the limit $p=0$ and $t_{\text{Co}}=0$ (Fig. 2, bottom).

There are then two components in $\Delta G(t_{\text{Co}})$. A constant offset determines the channeling contribution, and a free-electronlike, exponentially activated contribution determines the spin-dependent scattering contribution. The indicated contribution to GMR from channeling is sizable for the three low-index orientations, but is apparently somewhat lower for (110). A non-negligible channeling contribution is thus plausible for randomly oriented, polycrystalline structures.

III. PROPOSED EXPERIMENTAL TECHNIQUE

The different thickness dependencies of spin-dependent scattering and channeling contributions to GMR suggest a simple technique to isolate $\Delta G_{\text{chan}}$ in measurement. $\Delta G_{\text{chan}}$ is thickness independent, expressed as a constant offset to the experimental $\Delta G(t_{\text{Co}})$. For very strong surface diffuse scattering ($p_{\text{top}}=0$), $\Delta G_{\text{SDS}}$ is nearly zero in the limit of zero Co thickness. Thus the channeling contribution to GMR may be isolated in the zero-thickness limit of $\Delta G(t_{\text{Co}})$ if top surface specularity is fully suppressed. In situ magnetoconductance measurement is ideally suited for this purpose. We show sample in situ data which support the possibility of a sizable channeling contribution in NiO/Co/Co spin valves, and discuss how manipulation of $p_{\text{top}}$ is essential to isolate channeling.

Figure 3 shows a typical in situ magnetoconductance measurement for a NiO/Co(30)/Ru(6)/Co(20)/Cu(30 Å)/Co(t) spin valve on thermally oxidized silicon, taken at ambient temperature. The film is expected to be...
polycrystalline without strong preferred orientation. Magnetococonductance is measured at 0.35 Å intervals during pauses in UHV sputter deposition. The experimental data are compared with model calculations for $\Delta G_{SDS}$ “randomly oriented” Co(20)/Cu(30 Å)/Co(t), averaging (100) and (111) calculations in even proportions. A constant offset to all model curves of $\Delta G = +0.67 \text{m}\Omega^{-1}$ is introduced, representing a possible channeling contribution to GMR.

In the experiment shown, the offset in $\Delta G_{\text{Co}}$ cannot be uniquely identified with the channeling contribution $\Delta G_{\text{chan}}$. Figure 3 shows that finite top surface specularity $p_{\text{top}} = 0.25$ introduces a sizable offset into $\Delta G_{\text{Co}}$. Finite specularity may then be the source of the offset in the data shown. $p_{\text{top}} = 0$ provides the best reproduction of the $\Delta G$ size effect, however, and the agreement between experiment and the model is surprisingly good, considering that the SDS parameters from Ref. 9 have not been adjusted.

Unambiguous measurement of $\Delta G_{\text{chan}}$ will therefore require control of surface specularity $p$ during in-situ measurement. Schumacher has shown that electronic surface specularity of Ag films can be manipulated directly during deposition by temperature cycling. The RHEED-measured vacuum-side specularity was found to correlate well with the measured film-side specularity $p$. If specular reflections may be quenched at an atomically rough surface, $\Delta G_{\text{chan}}$ can be found straightforwardly. Controlled experiments of this nature will be useful to isolate the channeling contribution in Co/Cu/Co.

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151040, 1633, and 16400 k-points were used for (100), (111), and (110) orientations, respectively. Convergence was verified to within 5% using 6000 k-points in the (111) orientation. The choice of current direction is unimportant, as calculated values are isotropic in (100) and (111) and only weakly anisotropic in (110) trilayers.

16The transmissivity between the reduced second Cu band and first majority Co band shown for (110) is negligible.