The Influence of Defects on Electrical Transport in Magnetic Multilayers

J. Kudrnovsky, V. Drchal, I. Turek, C. Blaas, P. Weinberger, and P. Bruno

The transmission matrix approach was used to evaluate the perpendicular magnetotransport in metallic multilayers on an ab-initio *level. The spin-polarized, surface Green function technique was employed within the framework of the tight-binding, linear muffin-tin orbital method. The effect of impurities was included in terms of lateral supercells with random arrangements of two types of atoms. This approach treats both the ballistic and the diffusive regimes of magnetotransport on equal footing. The method was also applied to face-centered-cubic-based Co/Cu/Co(001) trilayers.*

INTRODUCTION

Transport properties of layered materials, particularly magnetic multilayers, are of great technological interest. The phenomenon of giant magnetoresistance (GMR) is promising for its applications, such as in nonvolatile magnetic random-access memories in the information technology industry or as reading heads and various kinds of sensors in the recording and car industries, respectively. Thus, transport in layered materials has been the subject of intensive theoretical and experimental investigations, particularly in view of the discovery of GMR in metallic multilayers.[1]

Most of the measurements to date are reported for current-in-plane (CIP) geometry,[2] since the current-perpendicular-to-plane (CPP) geometry[3] is experimentally more challenging. From a theoretical point of view, CPP transport is interesting because of the obvious role played by interfaces, its close relation to tunneling across an insulator or vacuum, and its relation to a semiclassical view of ballistic transport.[4]

The GMR effect has been observed mostly in the diffusive transport regime in which the mean free path is much smaller than the dimension of the so-called active part of the multilayer system (i.e., the whole system, with the exception of the leads). In the ballistic regime, the mean free path is larger than the dimension of the active part of the multilayer system.

Spin-dependent scattering at ideal interfaces between magnetic and nonmagnetic layers—intrinsic potential scattering—is usually considered the origin of GMR in the ballistic regime.[4] In the diffusive regime, GMR is thought to originate from spin-dependent scattering of impurities in the bulk and/or at interfaces between the magnetic slabs and the spacer (extrinsic defects). It should be noted that in real multilayers dislocations or stacking faults also occur, and magnons and phonons can cause dynamical perturbations (for finite temperatures). While in the limiting cases of the strong diffusive regime and the ballistic regime simplifications can be made, a real multilayer system usually represents a mixture of intrinsic and extrinsic defects.

Ab initio calculations of GMR are still rather rare. One such calculation method is solving the Boltzmann equation applied to multilayers.[5] The second method is a Kubo-Greenwood approach generalized to layered systems in terms of the layer Korringa-Kohn-Rostoker (KKR) method[6] as well as in terms of the relativistic spin-polarized screened KKR method,[7] neglecting vertex corrections with respect to the configurational average of the products of two single-particle Green functions. Both approaches can, at least in principle, be used for CIP and CPP. Alternative theoretical approaches applicable to the CPP transport are based on the Landauer-Büttiker formulation and its variants,[8] such as a nonequilibrium Green function method[9] or a transmission matrix formalism,[10–12] and were implemented within an empirical tight-binding method based on surface Green functions.

Such an approach was formulated within the first principles, tight-binding, linear muffin-tin orbital (TB-LMTO) method for a general stacking of nonrandom layers (ballistic transport). This formulation was then extended to the case of lateral two-dimensional supercells within each disordered atomic layer and with random occupation of supercell sites by two kinds of atoms (a substitutionally disordered binary alloy). The usefulness of such an approach has recently been illustrated for the case of a single-band tight-binding model.[13]

MAGNETOTRANSPORT

The magnetic multilayer system (the spin valve) consists of nonrandom, semi-infinite left (L″) and right (R) leads sandwiching an active part of the sample consisting of a left and a right magnetic slab of a finite thickness separated by a nonmagnetic spacer of varying thickness. The active part of the sample consists of N layers. It should be noted that left and right leads and magnetic slabs can consist of different metals. In practical realizations, the orientation of magnetic moments in one magnetic slab is fixed by a strong magnet (exchange layer), while orientations of magnetic moments in the other slab can be changed by an external magnetic field. Thus, there can be two possible orientations of magnetic moments in magnetic slabs of a spin valve—the ferromagnetic (F or the parallel) and the antiferromagnetic (AF or the antiparallel).

In principle, atomic layers can be viewed in terms of n × n supercells (n × n two-dimensional complex lattice). In order to describe disorder, it is then necessary to

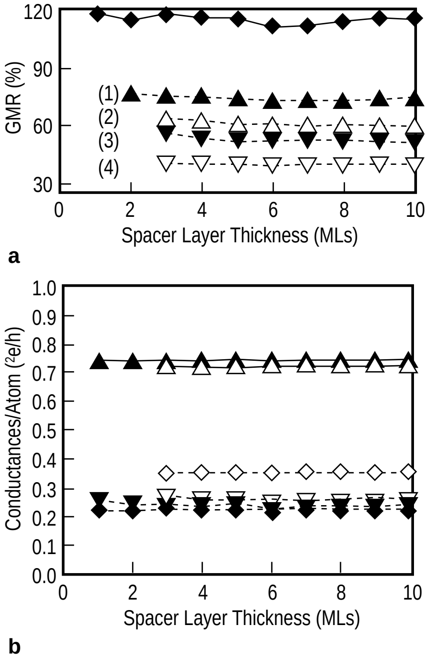

Figure 1. A comparison of trilayers with 15% interdiffused interfaces with ideal Co$_5$/Cu$_s$/Co$_5$ trilayers sandwiched by semi-infinite copper leads as a function of the spacer thickness s showing (a) magnetoresistance ratio (◆—ideal trilayer; ▲—one of the inner interfaces interdiffused; △—both inner interfaces interdiffused; ▼—two inner and one outer interfaces interdiffused; ▽—all four interfaces interdiffused) and (b) conductances per atom for the ferromagnetic ↑ spin (▲), ferromagnetic ↓ spin (▼), and antiferromagnetic configuration (◆). Full symbols refer to an ideal trilayer, empty symbols to a trilayer with all interfaces interdiffused.