Magnetic structure at copper–permalloy interfaces

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First principles local spin density calculations of the magnetic structure of interdiffused Cu/Py multilayers were performed. It was possible to solve the Kohn–Sham [Phys. Rev. **140**, A1133 (1965)] equations for both canted and collinear magnetic arrangements to a high level of convergence. We found multiple, metastable, noncollinear magnetic structures that showed a reduced contribution to the saturation magnetization consistent with roughly one ''magnetic dead'' layer per interface. These canted interface layers were stable with respect to collinear interfaces by about 2 mRy per atom at the interface. The calculated noncollinear total spin magnetic moments as a function of the number of Py layers were in good agreement with the experiment. © *1999 American Institute of Physics.* [S0021-8979(99)73708-4]

I. BACKGROUND

A giant magneto resistance (GMR) spin valve consists of two ferromagnetic layers separated by a thin layer of nonmagnetic metal. These three layers are mounted on an antiferromagnetic substrate that pins the moment direction in the adjacent ferromagnetic layer. There can be a large change in the electrical resistivity when an external magnetic field flips the orientation of the magnetization of the free layer.

Spin valves have possible application in magnetic read heads, magnetic sensors, and nonvolatile magnetic memory. The magnetically soft $Ni_{0.8}Fe_{0.2}$ solid solution known as permalloy, Py, is a leading candidate for the ferromagnetic material. Cu or Cu alloys are common choices for the nonmagnetic layer. The GMR ratio depends not only on the choice of materials but also on their thickness and on the details of the interfaces. For example it has been observed that the placement of less than a monolayer of Co at the ferromagnet–metal interface significantly improves the GMR ratio in Py/Cu/Py spin valves.[1]

The importance of the interface is also evident in the reduction of GMR ratios caused by annealing.[1] This reduction is usually ascribed to anneal induced interdiffusion at the interfaces. Also associated with interdiffusion are so-called magnetically dead layers. It is observed that there is a minimum number of atomic planes of magnetic material below which the magnetic planes have no magnetization.[1] Above this minimum number of atomic planes the moment increases linearly with the number of planes and the increase per plane is equal to the magnetization associated with a plane in the bulk magnetic material. It is known that magnetically dead layers are very detrimental to GMR. It is therefore important to understand this phenomenon.

II. MODEL CONSTRUCTION

The procedure used to construct configurations has been described previously[2] and will therefore only be reviewed here. The underlying concentration profiles are evolved from N perfect [111] atomic planes of Ni embedded in Cu. Although the process of atomic interchange during deposition involves several interchange mechanisms we make the simplifying assumption that Ni and Cu site occupations evolve according to the diffusion equation. The instantaneous configuration is a function of only the product of the time and the hopping frequency, $t\omega_d$. The saturation magnetization associated with a configuration can be calculated within the local spin density approximation at zero temperature or according to a simple model in which the moment on a Ni atom depends on its local concentration in the same way that the average Ni moment varies with concentration in the solid solution at the temperature of interest. Armed with the moment as a function of $t\omega_d$ we can fix the value of $t\omega_d$ by requiring that the number of magnetically dead layers agrees with the experiment.

Gurney *et al.*[3] found that at room temperature Cu/Ni/Cu has five magnetically dead layers; this fixed the only parameter in the simple diffusion model which then becomes applicable for any number of Ni atomic layers. We assumed that Cu, Ni, and Fe have similar diffusion constants, therefore, we simply replaced Ni by Fe at random in the Cu/Ni/Cu model to arrive at a model for Cu/Py/Cu. To recap, we started with five perfect Ni layers in Cu and let the Cu and Ni diffuse until the calculated moment went to zero. This specified how long to let model configurations diffuse for an arbitrary number of Ni layers. Following the assumption that Fe diffuses at the same rate as Ni we also constructed configurations corresponding to the deposition of arbitrary amounts of Py. This model can only be valid if Py and Ni samples were sputtered under the same conditions of ion energy, substrate temperature, etc.

Zhou and Wadley[4] have also obtained atomic structures, but by atomic simulation of vapor deposition of Ni layers in Cu. Their simulated concentration profile closely resembles

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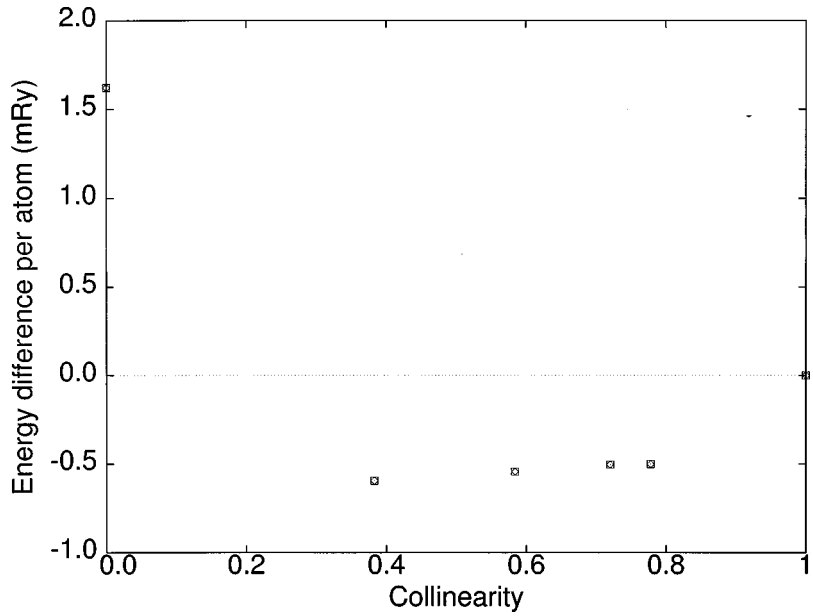

FIG. 1. The energy per atom for a 250 atom model of four atomic planes of Py interdiffused in Cu is shown for several levels of collinearity. The energy zero is the collinear state.

that from the simple diffusion model. Magnetic moments for the simulated model calculated with the locally self-consistent multiple scattering, LSMS[5] method and values calculated with the layer Korringa–Kohn–Rostoker (KKR)[6] for the diffusion model agree with each other and with experiment.[7] The consistency of these results convinced us that the diffusion model gave a reasonable model for Ni–Cu interfaces.

III. RESULTS

We extrapolated from Cu/Ni/Cu structures to Cu/Py/Cu structures by randomly replacing 20% of the Ni atoms by Fe atoms. If this is a valid procedure the calculated magnetization should agree with measured values. The saturation magnetization of Cu/Py/Cu spin valves was calculated with the (LSMS), (local interaction zone of 57 atoms), as a function of Py thickness and compared to experiment. Obviously, the magnetization at zero Py thickness is zero and at infinite thickness the derivative of the moment with Py thickness is just the magnetization of a layer of bulk Py. In addition to these two trivial data points we constructed two samples, one with nominally two layers and one with nominally four layers of Py. The first sample consisted of eight [111] hcp layers each with 25 atoms; the second sample had ten [111] hcp layers each with 25 atoms. Periodic boundary conditions were used.

In the course of trying alternative methods for iteratively solving the Kohn–Sham equations for the four Py layer case we obtained four different metastable magnetic structures for the same atomic configuration. In Fig. 1 the energies of these

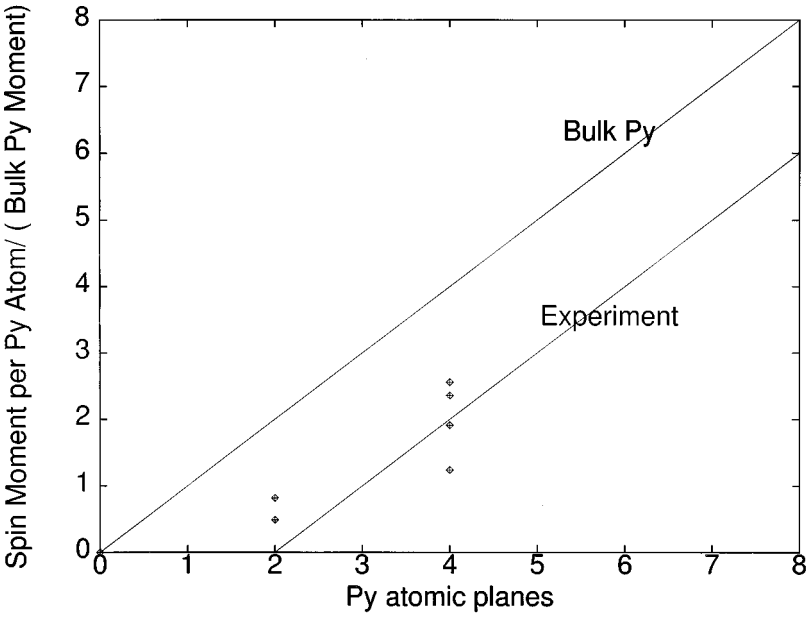

FIG. 2. Total spin magnetization per Py atom in the model as a function of the number of atomic planes of Py embedded in Cu. Values are shown for several metastable magnetic configurations. The moments are given in terms of the moment per Py atom in bulk Py.

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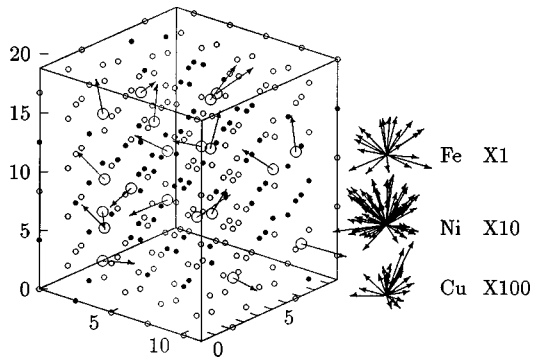

FIG. 3. Atomic positions and site magnetic moments for one magnetic configuration of four atomic planes of Py interdiffused into Cu. The distances are in angstroms and the moments are in Bohr magnetons. The small filled circles represent Ni, the small open circles represent Cu, and the large open circles represent Fe. All Fe moments, as well as. Ni moments greater than $0.15\mu_B$ and Cu moments larger than $0.015\mu_B$ are depicted to the right-hand side with the indicated multiplying factors.

metastable magnetic structures are plotted versus the collinearity. Energy is measured relative to the energy of the collinear case. We define the collinearity:

$$c=\frac{x-x_{\text{random}}}{1-x_{\text{random}}}, \tag{1}$$

where

$$x=\left|\frac{\sum_{i=1}^{N}\mathbf{m_i}}{\sum_{i=1}^{N}m_i}\right|, \tag{2}$$

$\mathbf{m_i}$ is the vector magnetic moment on site i, and N is the number of atoms in the unit cell. The value of x_{random} is found by averaging x over many sets of moment directions chosen randomly but with the moment magntudes kept fixed at the values appropriate for the magnetic configuration under investigation. As the number of atoms in the unit cell increases, the value of x_{random} goes to zero. This definition adjusts for the fact that a small number of moments randomly oriented will have a nonzero value of x even though the infinite system being modeled would have a zero value of x if the moments were randomly oriented. We measure the collinearity using the random case as a reference. Also shown is the energy of the sample when the iteration proceeded from the initial state with randomized moment directions and the moments were not allowed to change direction. This magnetic state has roughly zero collinearity. The fact that the random configuration has an appreciably higher energy than the metastable or collinear configurations demonstrates that the correlation among the moment directions was important in stabilizing the noncollinear structure. The most significant result was that the collinear state was not stable; there was some noncollinearity due to interdiffusion at the interface.

The plot in Fig. 2 of the magnetization as a function of deposited Py layers is consistent with experiment.[2] It is difficult to make definitive statements about the agreement because we have performed the calculations for only one atomic configuration at each of the Py layer thicknesses and we cannot do a full search for all metastable magnetic configurations. We infer from these calculations that other atomic configurations and other metastable magnetic structures would fall roughly in the range of those that we have thus far calculated. The magnetic structure corresponding to the lowest degree of collinearity for the four Py layer case is shown in Fig. 3. There appear to be pairs of moments that are ferromagnetically aligned while others have a canted relationship. These correlations are preserved from one metastable state to another.

IV. CONCLUSIONS

We have demonstrated that diffusion at the interface between Py and Cu results in noncollinear moments. We found multiple metastable magnetic configurations. The agreement between measured and calculated magnetization for the limited set of solutions obtained leads us to conclude that the canting of the Fe moments and a reduction of the magnitude of the Ni moments at the interface is responsible for the measured ''magnetically dead'' layers.

As discussed by Butler *et al.*[8] the effect of placing a small amount of Co at the interface can dramatically increase the collinearity. This Co induced increase in collinearity is consistent with improved GMR ratios and greater resistance to the detrimental effect on GMR ratios of annealing. Calculations of this type appear to provide a very promising tool for the design of interfaces. The benefit may, however, be limited because of the presence of multiple metastable magnetic structures. Furthermore, the computing resourses required to perform calculations of this type on the large number of atoms needed to model interfaces will restrict the number of configurations that can be studied.

ACKNOWLEDGMENTS

Work at Oak Ridge was sponsored by the Division of Materials Sciences Office of Basic Energy Sciences under Contract No. DEAC05-96OR22464 with Lockheed Marietta Energy Research Corporation and by the Defense Advanced Research Projects Agency.

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