Atomistic Modeling of the Interlayer Coupling Behavior in Perpendicularly Magnetized $L1_0$-FePt/Ag/$L1_0$-FePt Pseudo Spin Valves

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An atomistic model based on a classical spin Hamiltonian and a Landau–Lifshitz–Gilbert (LLG) equation was utilized to simulate and gain understanding of the magnetic, interfacial, and reversal properties of perpendicular anisotropy $L1_0$-FePt/Ag/$L1_0$-FePt pseudo spin valves, with different interfacial roughness, representing the experimentally observed behavior of the interface where the Ag spacer layer was postannealed at different temperatures. Simulation results showed that the influence of the Ag spacer on the independent switching of the FePt layers became stronger with a greater degree of interlayer mixing under higher temperature treatment. This was the result of an increased magnetic polarization of Ag with a decrease in Ag spacer thickness. Furthermore, with greater intermixing the magnetization reversal of the harder fixed FePt layer also changed from a coherent reversal process to one which took place via nucleation and propagation of reversed domains.

***Index Terms*—Ag, atomistic model, FePt, intermixing, pseudo spin valves.**

I. Introduction

RECENTLY, the giant magnetoresistance (GMR) and tunneling magnetoresistance (TMR) with perpendicular anisotropy have received more attention due to the intrinsic advantages over in-plane anisotropy for their applications in high-density recording and spin torque transfer magnetoresistive random access memory (MRAM) [1], [2]. Pseudo spin valves (PSVs) present an alternative to standard spin valves by utilizing different coercivities of the magnetic layers to control the switching behavior [3]–[5]. In recent experiments, PSVs with the structure MgO substrate/$L1_0$-FePt(20 nm)/Ag(2.5 nm)/$L1_0$-FePt(5 nm) were fabricated [6]. The Ag spacer layer was prepared under various postannealing temperatures of 300°C, 400 °C, and 500 °C. Postannealing affects the quality of the $L1_0$-FePt/Ag interface and defect concentration in the bulk layers which are of paramount importance to GMR [7]–[9]. In this work, an atomistic spin model was utilized to simulate and gain understanding of the magnetic, interfacial, and reversal properties of these fabricated PSVs.

II. Simulation Model

In this atomistic spin model, the energies of the system of interacting spins are described by a classical spin Hamiltonian of the form

$$\mathcal{H} = -\Sigma_{ij} J_{ij} S_i S_j - \Sigma_i K_i S_z^2 - \Sigma_i \mu_i H S_i. \tag{1}$$

The first term describes the exchange coupling between the two neighboring spins i and j, where J_{ij} is the exchange constant between the two spins and S_i *and* S_j are the spin moments of i and j, respectively. The second term describes the magnetocrystalline anisotropy of the spin, where K_i is the anisotropy energy per atom. The last term is a Zeeman constant which represents the interaction of an externally applied field H with the spin system, where μ_i is the magnetization of each atom.

The dynamics of the spin system are described by the Landau–Liftshitz–Gilbert (LLG) equation with Langevin dynamics

$$\frac{\partial S}{\partial t} = -\frac{\gamma}{(1+\lambda^2)}\left[S \times H + \lambda S \times (S \times H)\right] \tag{2}$$

where γ is the gyromagnetic constant, λ is the damping constant, and H is the effective magnetic field obtained from the derivative of spin Hamiltonian and an additional white noise term, $H = -(1/\mu_i)(\partial H/\partial S) + \zeta_i$.

The FePt layers were simulated as a generic ferromagnet with a Curie temperature (T_c) of 800 K, and uniaxial magnetocrystalline anisotropies (K_u) of 1.1×10^6 J/m^3 and 2.2×10^6 J/m^3 for the top and bottom layers, respectively, representing different degrees of $L1_0$ high anisotropy phase ordering. The Ag spacer layer was simulated as a paramagnet with a T_c of 8 K. The paramagnetic behavior of the spacer at temperatures greater than 8 K replicated the physical behavior of induced order near the FePt surface, while having no intrinsic order. Experimentally, the PSVs were made up of layers of continuous thin films. In this model, a vertical slice with dimensions of $5\times 5 \times 27.5$ nm^3 was simulated, having the correct layer thicknesses but a much smaller lateral dimension.

Due to the high-temperature fabrication conditions, diffusion between the different layers was expected to take place. In this atomistic model, the interlayer diffusion was controlled by the introduction of the following function for each material:

$$\tanh\left(\frac{x}{aL}\right) \tag{3}$$

where x is a position within the PSV, a is the intermixing factor, and L is the total length of the PSV system (27.5 ± 1.5 nm). The larger the intermixing factor a, the greater would be the degree of intermixing at the FePt and Ag interface (see Fig. 1). In this model, the Ag and FePt layers were assumed to have the same diffusion rates. The intermixing factors of the top FePt/Ag interface (a_t), bottom FePt/Ag interface (a_b) and thickness of the Ag

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Fig. 1. Schematic illustration of the dependence of Ag/FePt intermixing on intermixing factor a. Absence of intermixing when $a = 0$ (solid line). The extent of intermixing increases with increasing value of a, when $a > 0$ (dashed line to dotted line).

TABLE I
MODELING PARAMETERS AND DATA

Sample	a_t	t/nm	a_b	Degree of induced magnetic ordering in Ag
300 °C	0.02	2.5	0.02	0.258
400 °C	0.02	2.0	0.025	0.357
500 °C	0.02	1.5	0.03	0.527

Intermixing factor of the top FePt/Ag interface (a_t), thickness of the Ag layer (t), intermixing factor of the bottom FePt/Ag interface (a_b) as well as the corresponding magnetic ordering generated in Ag for PSVs with Ag post annealed at 300 °C, 400 °C, and 500 °C.

layer (t) were varied to model the conditions within the PSVs, where the Ag spacer was subjected to different postannealing temperatures.

III. RESULTS AND DISCUSSION

The values of a_t, t, and a_b for the simulated PSVs with the Ag spacer postannealed at various temperatures are summarized in Table I. The a_t was assigned a value of 0.02 across the simulated samples as the top FePt layer in all the PSVs were deposited at a high temperature of 300 °C to attain $L1_0$ ordering. Ag is immiscible in FePt and the diffused Ag atoms would tend to reside along the high energy grain boundaries [10], [11]. As such, an increase in the postannealing temperature of Ag would lead to a greater degree of diffusion of the Ag atoms into the bottom FePt layer as well as the grain boundaries. This was represented by an increasing a_b and a diminishing t, respectively. Fig. 2(a) shows the simulated hysteresis loops of the PSVs with the Ag layer postannealed at 300 °C, 400 °C, and 500 °C. Decoupling between the top and bottom FePt layers was no longer present at a Ag postannealing temperature of 500 °C. Increasingly extensive bottom FePt/Ag interlayer diffusion with higher postannealing temperature resulted in a larger number of Ag atoms in contact with the FePt atoms. The magnetic moments of the surrounding FePt atoms would polarize the Ag atoms. The polarizing effect on Ag becomes greater with a larger degree of intermixing, which in turn exerts a greater influence on the switching of the FePt layers. An increase in the induced magnetic ordering of the Ag spacer was observed with increasing Ag postannealing temperature (Table I). This suggested that an increasingly polarized Ag spacer contributed to the increased effective exchange coupling between the FePt layers. Furthermore, diffusion of the Ag atoms to the grain boundaries at a higher Ag postannealing temperature gave rise to a reduced spacer thickness (see Fig. 3), which could have been too thin to bring about complete decoupling between the top and bottom FePt layers.

Although the simulated results were in good agreement with experimental data, where a thinner Ag spacer along with coupling behavior between the $L1_0$-FePt layers were observed at a

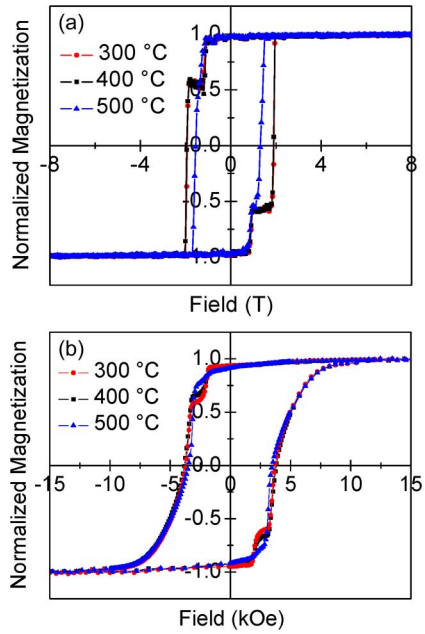

Fig. 2. Hysteresis loops of (a) simulated and (b) experimentally fabricated FePt/Ag/FePt PSVs with varying Ag postannealing temperatures of 300 °C, 400 °C, and 500 °C.

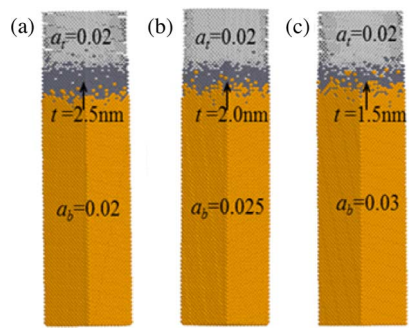

Fig. 3. Schematic illustration of simulated FePt/Ag/FePt PSVs with varying Ag postannealing temperatures of (a) 300 °C, (b) 400 °C, and (c) 500 °C.

postannealing temperature of 500 °C, the simulated hysteresis loops deviated slightly from the experimental one [Fig. 2(b)]. Complete magnetization reversal took place instantaneously at the coercive field, unlike that observed from experimental results. This was attributed to the small simulation dimensions in atomistic modeling in which focus was placed on a single grain rather than on a multiple grain structure observed experimentally. As such, intergrain exchange interactions within the FePt layers were neglected in this model. Furthermore, a perfect lattice model was assumed in the simulation whereas fabricated samples were unlikely to be defects free. Coercivity values obtained from simulation results were also much higher than experimental ones due to the smaller simulated sample dimension.

A rougher and more poorly defined interface was observed along with increasing intermixing factor (Fig. 3). Interfacial scattering and spin accumulation at the interface are of utmost importance to the magnetoresistance of the PSV structure. The atomically rough interface could have led to a greater degree of spin flipping and reduced spin accumulation, thus contributing to the decrease in GMR ratio with increasing Ag postannealing temperature, as observed experimentally.

The switching mechanism of the FePt layers in the PSVs post-annealed at 300 °C and 500 °C, in the presence and ab-

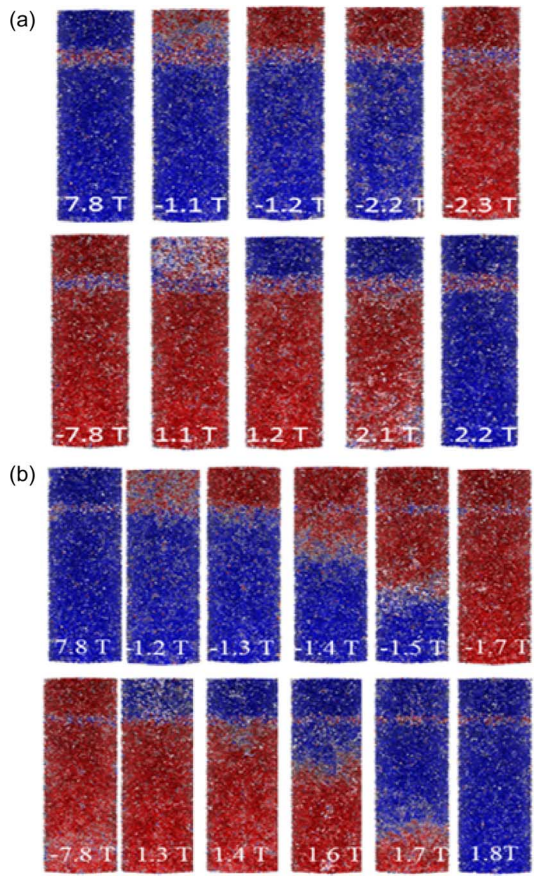

Fig. 4. Schematic representation of the magnetization state of Ag and FePt atoms at various applied field along the hysteresis loop for the simulated PSVs with Ag postannealed at (a) 300 °C and (b) 500 °C. Spin-up, spin-down, and in-plane magnetization are represented in blue, red, and white, respectively.

sence of interlayer decoupling respectively, was investigated by studying the magnetic moments of the FePt and Ag atoms at different stages of the hysteresis cycles. In both PSVs, all the FePt atoms possessed spin-up magnetization (blue) under a positive saturation field of 7.8 T [Fig. 4(a) and (b)]. The Ag atoms possessed a randomized combination of spin-up (blue), spin-down (red), and in-plane (white) magnetization due to its paramagnetic nature at 300 °C. In both cases, upon reaching the coercive field of the top FePt layer, in the range of 1.1–1.3 T, reversal occurred simultaneously and coherently and spin-down magnetization (red) of the top FePt layer was attained. On the other hand, reversal of the bottom FePt layer was different for the PSVs with different Ag spacer postannealed temperatures. For the case at 300 °C, coherent rotation of the bottom FePt, similar to that of the top FePt, was observed. When the Ag postannealing temperature increased to 500 °C, reversal of the bottom FePt became incoherent. Magnetization reversal began at the region where the bottom FePt layer was closest to the Ag spacer, followed by the subsequent propagation of reversed domains through the remaining portion. Based on the reversal schematic diagram in Fig. 4, the switching field of the bottom and top FePt layers occurred within a closer coercivity range when the Ag spacer was postannealed at 500 °C compared to that at 300 °C. Exchange coupling between the FePt layers became more dominant at a higher postannealing temperature due to the thinner Ag spacer layer. As such, initial nucleation of reversed domains in the bottom FePt layer occurred under the assistance of exchange interaction with the top FePt layer. This took place at the region near the Ag spacer where exchange interaction was the strongest due to closer proximity between the FePt layers. At the same time, the increasing presence of reversed polarized Ag near the interface of the bottom FePt layer could also have contributed to the initial reversed domains formation at this region.

IV. Conclusion

An atomistic spin model was used to simulate perpendicular anisotropy $L1_0$-FePt/Ag/$L1_0$-FePt PSVs, with the Ag spacer layer postannealed at various temperatures of 300 °C, 400 °C, and 500 °C. The effects of interlayer diffusion with a higher postannealing temperature of Ag spacer layer were modeled with a smaller Ag spacer layer thickness and larger intermixing factor. With an increase in postannealing temperature to 500 °C, the simulated hysteresis loop indicated a loss of decoupling between the magnetic layers of the PSV. This was in good agreement with experimental observations of the PSVs. An increasingly atomically rougher interface resulted from the higher postannealing treatment. For the Ag postannealing temperature of 300 °C, magnetization reversal of the soft and hard FePt layers occurred coherently. However, a different set of reversal mechanism was observed for the bottom FePt layer when the Ag spacer was postannealed at 500 °C, in which reversal took place through reversed domains formation and propagation.

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References

[1] J. G. Zhu, "Magnetoresistive random access memory: The path to competitiveness and scalability," *IEEE. Trans. Magn.*, vol. 96, pp. 1786–1798, 2008.
[2] J. M. Slaughter, "Materials for magnetoresistive random access memory," *Annu. Rev. Mater. Res.*, vol. 39, pp. 277–296, 2009.
[3] F. Russo, G. Carapella, V. Granata, N. Martucciello, and G. Costabile, "Pseudo spin-valves with Al or Nb as spacer layer: GMR and search for spin switch behavior," *Eur. Phys. J. B.*, vol. 60, pp. 61–66, 2007.
[4] S. Tehrani, M. Durlam, M. DeHerrera, and E. Chen, "High density pseudo spin valve magnetoresistive RAM," in *Proc. Int. NonVolatile Memory Technol. Conf.*, 1998, vol. 56085, pp. 43–46.
[5] A. Paul, T. Damm, D. E. Burgler, S. Stein, H. Kohlstedt, and P. Grunberg, "Optimizing the giant magnetoresistance of NiFe/Cu/Co pseudo spin-valves prepared by magnetron sputtering," *Appl. Phys. Lett.*, vol. 82, pp. 1905–1907, 2003.
[6] P. Ho, G. C. Han, R. W. Chantrell, R. F. L. Evans, G. M. Chow, and J. S. Chen, "Perpendicular anisotropy $L1_0$-FePt based pseudo spin valve with Ag spacer layer," *Appl. Phys. Lett.*, vol. 98, 2011, 132501.
[7] E. M. Ho, A. K. Petford-Long, and A. Cerezo, "The effect of interfacial regions on the giant magnetoresistance in as-grown and annealed Fe/Cr MLFs," *J. Magn. Magn. Mater.*, vol. 192, pp. 431–442, 1999.
[8] G. J. B. Rodriguez, L. G. Pereira, M. G. M. Miranda, A. B. Antunes, and M. N. Baibich, "Magnetotransport and coupling in nanostructured Co/Ag thin films," *J. Magn. Magn. Mater.*, vol. 214, pp. 78–84, 2000.
[9] H. Laidler, B. J. Hickey, T. P. A. Hase, B. K. Tanner, R. Schad, and Y. Bruynseraede, "Effect of annealing on the roughness and GMR of Fe/Cr multilayers," *J. Magn. Magn. Mater.*, vol. 156, pp. 332–334, 1996.
[10] S. Thongmee, B. H. Liu, J. Ding, and J. B. Yi, "Diffusion induced columnar structure, high perpendicular anisotropy and low transformation temperature in thick FePt films," *Thin Solid Films*, vol. 518, pp. 7053–7058, 2010.
[11] S. C. Chen, P. C. Kuo, A. C. Sun, C. Y. Chou, Y. H. Fang, and S. Y. Kuo, "Microstructure and coercivity of granular nanocomposite FePt-Ag multilayer films," *IEEE Trans. Magn.*, vol. 41, pp. 3340–3342, 2005.