Magnetic structure of domain walls confined in a nano-oxide layer

Katsuyoshi Matsushita, Jun Sato and Hiroshi Imamura
Nanotechnology Research Institute (NRI),
Advanced Industrial Science and Technology (AIST),
AIST Tsukuba Central 2, Tsukuba, Ibaraki 305-8568, Japan.

Abstract—In the recent years, a spin-valve was developed with a current-confined-path structure consisting of a non-oxide-layer (NOL). We analyze magnetic structures of the current-confined-path in the nano-oxide layer sandwiched between ferromagnetic electrodes and clarify the dependency of the magnetic structure on the shape and size of the current-confined-path. Our results of stiffness energy density and thermal stability shows that we should fabricate a CPP spin-valve with narrow current-confined-paths with large aspect ratio and strong constriction in order to enhance the MR ratio.

Index Terms—CPP-GMR, current-confined-path, micromagnetic simulation, domain wall

GEOOMETRICALLY confined domain walls of nanometer size contacts have attracted enormous attention of researchers because of its possibility in applications to future spintronic devices [1, 15]. In the last decade much effort has been devoted to study magnetoresistance (MR) of domain walls in atomic wires. One of main obstacles to applications of the atomic wires is mechanical stability. For example, Chopra et al. [11] reported that a Co atomic wire that shows 300% MR ratio is stable for periods of up to as short as 2-3 mins. Recently, Fuke et al. fabricated a spin-valve of magnetic nanomultilayers with a current-confined-path structure consisting of a nano-oxide-layer (NOL) with a lot of fine holes filled with ferromagnetic metal [14, 15]. The holes of an NOL are very stable and its typical size is as small as a few nanometers. They showed that MR ratio of the spin-valves increases with increasing a value of resistance area product, which means that the MR ratio due to the geometrically confined domain walls is enhanced for the narrow metallic channels. In order to understand these experimental results, it is important to study magnetic structures of the domain walls confined in the NOL. However, it is very difficult to observe the magnetic structure of the domain walls directly by using a scanning probe microscope or optical techniques because the domain walls are confined in the NOL.

The micromagnetic simulation technique provides a powerful tool for studying magnetic properties of such geometrically confined domain walls [6]-[13]. Magnetic structures of the confined domain walls are investigated in atomic wire bridges with crystalline anisotropy by several groups [6]-[10]. However the effect of the crystalline anisotropy on magnetic structures should be small for the NOL spin-valve [14, 15] where the size of the domain walls is of the order of a few nanometers. Although a few simulations for contacts without crystalline anisotropy have been reported in [11]-[13], a certain careful simulation where the real shape of the current-confined-path in the NOL spin-valve [14, 15] is taken into account is needed to design the highly sensitive magnetoresistive devices.

In the present paper, we study shape dependence of magnetic structures of current-confined-paths in the NOL by using the micromagnetic simulation. We evaluate stiffness energy density of the magnetic structures in the NOL sandwiched between two magnetic layers of which magnetizations are aligned antiparallel to each other. We can estimate the effective thickness of the geometrically confined domain wall from the calculated stiffness energy density. We show that a narrow current-confined-path with large aspect ratio and strong constriction is required in order to enhance the MR ratio.

We employ a spin model on the simple cubic lattice, which is defined by the Hamiltonian,

\[
\mathcal{H} = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + K_d \sum_i \vec{S}_i \cdot \left( \int d\vec{r} \vec{D}(\vec{x}_i - \vec{r}) \cdot \vec{S}(\vec{r}) \right) + K_u \sum_i \left( 1 - (\vec{e}_i \cdot \vec{S}_i)^2 \right) + \sum_i \vec{h}_i \cdot \vec{S}_i. \tag{1}
\]

The local values at the \(i\)-th site, \(\vec{S}_i, \vec{e}_i, \vec{h}_i\) denote an unit vector representing a classical Heisenberg spin, a coordinate, an unit vector aligned in a direction of crystalline anisotropy and an applied magnetic field, respectively. The first term in the right hand side of (1) is the exchange stiffness energy between spins at nearest neighbor sites. The exchange coupling constant is denoted by \(J\). The value of \(J\) is related to exchange stiffness constant, \(A\), and a lattice constant, \(a\), as \(J = 2aA\).

The second term is the dipole-dipole interaction energy. The tensor function, \(\vec{D}(\vec{x})\), is expressed as,

\[
\vec{D}(\vec{x}) = \frac{1}{4\pi} \frac{1 - 3\vec{e}_z \otimes \vec{e}_z}{|\vec{x}|^3},
\]

where \(\vec{e}_z = \vec{x}/|\vec{x}|\). The dipole-dipole coupling constant, \(K_d\), is equivalent to \(a^3 \mu_0 M_s^2/2\), where \(M_s\) and \(\mu_0\) are the saturation magnetization and vacuum permeability, respectively. In order to deal with the dipole-dipole interaction in the NOL spin-valve, we adopt a finite element - boundary element (FEM-BEM) hybrid method [17]. In the evaluation of the stray field coming from the dipole-dipole interaction, spins at lattice...
The finite element mesh of the current-confined-path in the NOL spin-valve is shown. The shape of the current-confined-path is deformed to a hyperboloid parameterized by two ratios, \(d/h\) and \(d_c/d\), where \(d\), \(d_c\), and \(h\) denote the diameter of the center, that of the bottom and height, of the current-confined-path, respectively.

points are extrapolated to that in the whole region in the NOL, \(S(\vec{r})\).

The third term is the crystalline anisotropic energy. We neglect this term in the present calculation because the characteristic length determined by the crystalline anisotropy is a few-tens of nanometers and therefore the effect of the crystalline anisotropy on the magnetic structure of the geometrically confined domain wall of a few nanometer size must be very small.

The forth term is the Zeeman energy due to the applied magnetic field. We also neglect the Zeeman energy in the present calculation and the direction of the magnetizations in the top and bottom electrodes are determined by the boundary conditions. The boundary conditions we use are the following: \(S_t^x = 1\) on top and side surfaces of the top electrode and \(S_t^y = 1\) on bottom and side surfaces of the bottom electrode. On the other surface the boundary condition is free.

The system we consider is schematically shown in Fig. 1. The system is divided to a 3-dimensional lattice consisting of hexahedral finite elements. The number of elements in the top electrode is taken to be \(39 \times 39 \times 3 = 4563\). The bottom electrode is divided in the same way as in the top electrode. The number of elements in the \(z\)-direction in the contact is taken to be 9. The total number of the elements, which depends on the ratio \(d/h\), is of the order of \(10^4\). The shape of the contact is assumed to be a hyperboloid parameterized by two ratios, where \(d\) and \(d_c\) are the diameters, respectively, at the center and the bottom of the contact, and \(h\) is the height of the contact. The characteristic length determined by the competition between the exchange interaction \(\mathcal{H}_{ox}\) and the dipole-dipole interaction \(\mathcal{H}_d\) is the exchange length defined by,

\[
l_{\text{ex}} = \sqrt{\frac{A}{K_d}},
\]

which is of the order of a few nanometers for conventional ferromagnetic metals. We assume that \(l_{\text{ex}} = 2.8\text{nm}\) corresponding to the materials used in Fig. 1. The unit length of the system, \(a\), is taken to be \(\sqrt{K_d/J_{\text{ex}}}\) and the height of the NOL is \(h = 2\text{nm} (\sim 0.71\text{ex})\).

The classical Heisenberg spin system is embedded in the whole region as shown in Fig. 1. The spins obeys the Landau-Lifshitz-Gilbert equation,

\[
\frac{d}{dt} \vec{S}_i = \frac{\gamma}{1 + \alpha^2} \vec{S}_i \times \left\{ \frac{\partial \mathcal{H}}{\partial \vec{S}_i} + \alpha \vec{S}_i \times \frac{\partial \mathcal{H}}{\partial \vec{S}_i} \right\},
\]

where \(\gamma\) and \(\alpha\) are the gyromagnetic ratio and the Gilbert damping constant, respectively. The calculated ground states by the present simulation do not depend on their values. We simulates relaxation of the spins from various initial states by numerically solving the equation at zero temperature to obtain the ground state. The time integration is continued until a space- and time-averaged value of the torque exerted to the spins is of the order of \(10^{-8}\gamma J/(1 + \alpha^2)\). In the present simulation, further time-integration does not produce additional change of magnetic structures within the reachable time scale by our computers. The obtained lowest energy state by simulations started from three initial states is regarded as the ground state at each given set of parameters.

In the present simulation, by changing two ratios, \(d/h\) and \(d_c/d\), we investigate the systems in the range of \(0.8 < d/h < 4.0\) and for \(d_c/d = 0.25, 0.5, 0.75\) and 1.0. The obtained ground states are the Néel- and Bloch-wall like states as shown in Figs. 2(a) and 2(b), respectively.

The magnetic structure diagram is shown in Fig. 2(c). At small values of \(d/h\), the ground states are the Néel-wall like state. On the other hand the ground states observed at large values of \(d/h\) are the Bloch-wall like state. The similar results were obtained for atomic wires with a crystalline anisotropy by Coey et al. \[6\]. The result can be understood as follows: Our results show that the magnetic structures depend almost only on \(z\)-component of coordinates. Thus the exchange energy does not depend on whether the Bloch-wall or Néel-wall like structures \[6\] and we can discuss the energy of the states only by the dipole-dipole interaction energy. The dipole-dipole interaction energy on the surface of the contact, which decreases with increasing the aspect ratio, \(d/h\), gives a dominant contribution to the total energy of the Bloch-wall like state. On the other hand, the dipole-dipole interaction energy in the interior of the contact, which increases with increasing the aspect ratio, \(d/h\), gives a dominant contribution to the total energy of the Néel-wall like state. Therefore the Bloch-wall (Néel-wall) like state is preferred for the wide (narrow) contact as show in Fig. 2(c). As we increase the ratio \(d_c/d\), the dipole-dipole interaction on the surface of the contact increases but that in the interior of the contact decreases. Therefore the value of the aspect ratio \(d/h\) which determines the boundary between the Bloch- and Néel-like wall states is a decreasing function of the ratio \(d_c/d\).

Figs. 2(a)-(2 d) show the dependence of the stiffness energy density on the size and shape of the contact. The stiffness energy density is defined as

\[
E_{\text{ex}} \equiv \frac{J}{2K_{\text{ex}}} \int d\vec{r} \left( \nabla \cdot \vec{S}(\vec{r}) \right)^2,
\]

\[
\sim \frac{J}{2\alpha^2} \int_{z_{-} - a/2}^{z_{+} + a/2} dz \left| \nabla \theta(z) \right|^2,
\]

where \(\theta(z)\) denotes azimuthal angle for the Bloch-wall like
state and polar angle for the Neel-wall like state. \(v_i\) is total volume of elements near the \(i\)-th site. The last expression in (3) is justified for much small values of \(K_d/J\). In our simulation, value of \(K_d/J\) about 0.006 and thereby the approximation is also justified.

The stiffness energy densities of the narrow contacts are shown in Figs. 3(a) and 3(b). The stiffness energy densities are almost confined in the NOL and its spacial distribution can be controlled by changing the shape of the contact. Comparing the results shown in Figs. 3(a) and 3(b), one can see that the stiffness energy density of \(d_c/d = 0.5\) is much more concentrated at the center of the system than that of \(d_c/d = 1.0\). Since MR ratio increases with decreasing the thickness of the domain wall, we can expect a larger value of the MR ratio of the contact with \(d_c/d = 0.5\) than that with \(d_c/d = 1.0\).

The stiffness energy densities of the wide contacts are shown in Figs. 3(c) and 3(d). The stiffness energy densities stick out from the NOL and therefore the effective thickness of the domain wall is thicker than that for the system with the narrow contacts. As shown in Fig. 3(c), a strong concentration of the stiffness energy density appears around the surface of the contact with \(d_c/d=0.5\). Although a strong concentration of the stiffness energy density means that we have a thin domain wall around the surface, we cannot expect the large MR ratio because the other region with small stiffness energy density gives a small contribution to the MR ratio and acts as a parasitic resistance.

Finally, we discuss the stability of the ground states. The bistability of the Bloch and Neel-like structures is observed for almost all of the region of the parameters except for \(d_c/d = 0.25\) and \(d/h \leq 3\). Thus thermal instability is expected in those as discussed in [6, 7]. In our results, the energy difference between the Bloch- and Neel-wall like states is of the order of a few Kelvins at most. Although in wide contacts the energy difference between the Bloch- and Neel-wall like states increases with increasing system volume. If \(h\) is set at the typical experimental value of 2 nm [14], \(d\) should be a tens nanometers at least in order that the energy difference reaches room temperatures. However, as discussed before, we can not expect large MR ratios for such wide contacts. In the Neel-wall like states, we do not observe the excited Bloch state for \(d_c/d = 0.25\) and \(d/h \leq 3.3\) within our calculation accuracy. Therefore the narrow contacts with large aspect ratio and strong constriction has stable magnetization. The narrow contacts are a potential candidate of highly sensitive magnetoresistive devices because of their high magnetoresistance ratio as mentioned before.

In summary, we analyze magnetic structures of a current-confined-path in a nano-oxide layer sandwiched between ferromagnetic electrodes and clarify the dependency of the magnetic structure on the shape and size of the current-confined-path. Our results of stiffness energy density and thermal stability shows that we should fabricate narrow current-confined-path with large aspect ratio and strong constriction in order to enhance the MR ratio.

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