Thermal stability of geometrically confined domain wall structures

Munetaka Sasaki\textsuperscript{1}, Katsuyoshi Matsushita\textsuperscript{2}, Jun Sato\textsuperscript{2} and Hiroshi Imamura\textsuperscript{2}

\textsuperscript{1} Department of Applied Physics, Tohoku University, Sendai 980-8579, Japan.
\textsuperscript{2} Nanotechnology Research Institute (NRI), Advanced Industrial Science and Technology (AIST), AIST Tsukuba Central 2, Tsukuba 305-8568, Japan.
E-mail: msasaki@camp.apph.tohoku.ac.jp

Abstract. We investigate thermal stability of magnetic wall structure which is confined geometrically in a nano-contact. We measure free-energy as a function of magnetizations which characterize magnetic wall structures. Thermal stability is estimated from the free-energy barrier $F_b$ beyond which the system translates to another state. The typical value of $k_B^{-1}F_b$ is a few thousand Kelvin when the height of nano-contacts is 8 nm. The optimum shape of the nano-contact as magnetoresistance devices is clarified by examining the shape dependence of the free-energy barrier.

1. Introduction

Geometrically confined magnetic walls in ferromagnetic nano-scale contacts\textsuperscript{[1]} have been intensively investigated because of their applications to magnetoresistance (MR) devices [2, 3, 4, 5, 6, 7, 8]. One of important issues in the practical application of MR devices is to control thermal fluctuation of the magnetic structure. The thermal fluctuation which results from the Joule heating induced by the current conducting through the MR device must be inhibited because the thermal fluctuation of the magnetic structure induces a noise in the MR signal.

The thermal fluctuation of the magnetic structure of geometrically confined magnetic wall in ferromagnetic nano-contacts is suppressed by a potential barrier due to the dipole-dipole interaction\textsuperscript{[9, 10]}. The potential barrier is controllable by the size and the shape of nano-contacts. On the other hand narrow nano-contacts are desired because the MR signal increases as the radius of the nano-contact decreases. A fine-tuned narrow nano-contact, thereby, is needed to inhibit the thermal fluctuation and to keep the efficiency of the MR device. In the present paper we theoretically investigate the stability of the geometrically confined magnetic wall in nano-contacts at from room temperature to the transition temperature in order to clarify the proper design of ferromagnetic nano-contacts. We evaluate values of the potential barrier on some narrow nano-contacts by a Monte Carlo simulation and clarify the shape of the nano-contact which maximizes the potential barrier.
2. Model and Method

In the present work, we employ a spin model on the simple cubic lattice with a Hamiltonian

\[ \mathcal{H} = -J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + K_d \sum_{i<j} \frac{\mathbf{S}_i \cdot \mathbf{S}_j - 3(e_{ij} \cdot \mathbf{S}_i)(e_{ij} \cdot \mathbf{S}_j)}{|r_{ij}|^3} \quad (J > 0, K_d > 0), \]  

where \( \mathbf{S}_i \) is a classical Heisenberg spin with absolute value of unity, \( r_{ij} = r_i - r_j \), \( r_i \) is the position vector of a site \( i \) in the unit of the lattice constant \( a \), and \( e_{ij} = r_{ij}/|r_{ij}| \). The first term and the second term in the right hand side denote ferromagnetic exchange interactions and dipolar interactions, respectively. The sum of the exchange interactions runs over all the nearest-neighboring pairs. The value of \( J \) and that of \( K_d \) are given as

\[ J = 2aA, \quad K_d = J_s^2a^3/(4\pi\mu_0), \]

where \( A \) is the exchange stiffness constant in continuous limit, \( \mu_0 \) is the vacuum permeability and \( J_s \) is the saturation polarization. In this work, we use the value of \( A = 26 \text{ pJ/m} \) and \( J_s = 2.2 \text{ T} \), which are close to values of typical soft magnetic materials such as iron and cobalt. The transition temperature of this model is about 1,050 K if we assume that the atomic diameter of the material is 0.2 nm.

The shape of the model is shown in Fig. 1. The model consists of two electrodes and a constricted nano-contact in between. Classical Heisenberg spins are located at the center of each sphere. In order to simulate the experimental situation with a 180° wall, the spins in the dark gray spheres of the top electrode are fixed to (-1,0,0) and those of the bottom electrode are fixed to (+1,0,0), respectively. As shown in Fig. 1, the dark gray spheres are located at the five surfaces of each electrode. The other spins in the light gray spheres are free. Figure 2 shows the cross section of the model in the \( x-z \) plane containing the center. Since we consider the case that the dimensions in the \( x \) and \( y \) directions are the same, the cross section in the \( y-z \) plane has the same geometry. To examine shape effect, \( n_x \) is varied from 10 to 30 with fixing \( n_z \) at 10, where \( n_x \) is the number of spins in the \( x \) direction and \( n_z \) is that in the \( z \) direction (see Fig. 2). We also examine size effect by changing the lattice constant \( a \). The values of \( a \) we investigate are 0.2 nm, 0.4 nm and 0.8 nm. Therefore, the corresponding heights of the nano-contact \( l_z = n_z \times a \) are 2 nm, 4 nm and 8 nm, respectively. The height of nano-contacts in experiment is 2.5 nm[6].

In the present work, we use a new Monte Carlo method called Stochastic CutOff (SCO) method [11]. This method enables us to reduce computational time of dipolar interactions per one Monte Carlo step from \( \mathcal{O}(N^2) \) to \( \mathcal{O}(N \log N) \) without any approximation, where \( N \) is the number of spins. Firstly, this method is combined with simulated annealing to measure
maximum value of $k(l)$ (not shown), and found that the free-energy difference depends on
the contact described by the ratio $l_x/l_z$. The difference has a minimum around
$x(l) = 2$ is about $3 \times 10^4$ K. We also examined the case that $l_x/l_z = 1.0$ and $l_x/l_z = 2.0$.
This result is consistent with the result shown in Fig. 3(a). We performed such measurements for
four temperatures. The value of $k_B^{-1} |F_{\text{Néel}} - F_{\text{Bloch}}|$ at $l_x/l_z = 2$ is about 3,000 K. We also examined the case that $a = 0.4$ nm and $l_x/l_z = 4$ nm
(not shown), and found that the free-energy difference depends on $l_x/l_z$ in a similar way. The
maximum value of $k_B^{-1} |F_{\text{Néel}} - F_{\text{Bloch}}|$ for narrow contacts ($l_x/l_z \leq 2.5$) was about 400 K. Since

spin configurations at low temperatures. Secondly, this method is combined with a variant of
Wang-Landau method [12, 13] to measure free-energy as a function of magnetizations. Unlike
the original Wang-Landau method which calculates the density of states of energy, this variant
version of the method enables us to calculate free-energy.

3. Results

Figure 3 shows spin configurations obtained by simulated annealing. A Néel magnetic wall
is observed in the narrow contact ($l_x/l_z = 1.0$) and a Bloch magnetic wall is observed in the wide
contact ($l_x/l_z = 3.0$). We next measure the free energy $F(\beta; m_y, m_z)$ defined by

$$
\exp[-\beta F(\beta; m_y, m_z)] = C \text{Tr} \{\mathbf{S}_i\} \exp[-\beta \mathcal{H}(\mathbf{S}_i)] \delta(m_y - m_y^*) \delta(m_z - m_z^*) \mathbf{S}_i, \quad (3)
$$

where $\beta$ is the inverse temperature and $C$ is some constant. Note that the right hand side
of the equation is proportional to the probability that the state with magnetizations $(m_y, m_z)$
is observed. $m_\mu^*$ is the $\mu$-component of magnetization calculated from the contact part, i.e.,
$m_\mu^* \mathbf{S}_i \equiv (1/N') \sum_{\mu} \mathbf{S}_i^{(\mu)}$, where the sum $\sum$ runs over the spins in the contact part and $N'$
is the number of spins there. On the other hand, the trace in the right hand side runs over all the
free spins including those in the electrodes. Since the Bloch wall structure and the Néel wall
structure are characterized by $(m_y^*, m_z^*) = (c, 0)$ and $(m_y^*, m_z^*) = (0, c)$ respectively ($c$ is some
finite value), we can estimate the free-energies of these structures and the difference between
them by measuring $F(\beta; m_y, m_z)$.

As an example, $k_B^{-1} F$ for $l_x = l_z = 8$ nm is shown in Fig. 4. The free-energy is plotted as
a function of $(m_y, m_z)$ since it is symmetric with respect to $m_y$ and $m_z$. We see that Néel
magnetic wall is stable since the minimum of the free-energy is located around $(0, 0)$. This
result is consistent with the result shown in Fig. 3(a). We performed such measurements for
various values of $l_x$ at four temperatures $T = 945$ K, 735 K, 525 K and 315 K. The results are
summarized in Fig. 5. In this figure, $k_B^{-1} (F_{\text{Néel}} - F_{\text{Bloch}})$ is plotted as a function of $l_x$ for
the four temperatures. The value of $a$ is 0.8 nm and that of $l_x$ is 8 nm. We see that the free-energy
difference has a minimum around $l_x = 16$ nm. This result indicates that the shape of the nano-
contact described by the ratio $l_x/l_z = 2.0$ is optimum as MR devices since narrow nano-contact
with high free-energy barrier is desirable as mentioned in §1. The value of $k_B^{-1} |F_{\text{Néel}} - F_{\text{Bloch}}|$ at $l_x/l_z = 2$ is about 3,000 K. We also examined the case that $a = 0.4$ nm and $l_x/l_z = 4$ nm
(not shown), and found that the free-energy difference depends on $l_x/l_z$ in a similar way. The
maximum value of $k_B^{-1} |F_{\text{Néel}} - F_{\text{Bloch}}|$ for narrow contacts ($l_x/l_z \leq 2.5$) was about 400 K. Since

Figure 3. Spin configurations in the $x$-$z$ plane containing the center. The temperature is 315 K,
a = 0.8 nm and $l_z (= a \times n_z) = 8$ nm for both the figures, while $l_z (= a \times n_z)$ is 8 nm for Fig. 3(a)
and 24 nm for Fig. 3(b). The radius of the sphere at each spin is proportional to the magnitude
of the $y$-component of the spin.
Figure 4. $k_B^{-1}F(\beta;m_y,m_z)$ is plotted as a function of $(|m_y|,|m_z|)$. The temperature is 315 K, $a=0.8$ nm and $l_x=l_z=8$ nm.

Figure 5. The size $l_x$ and temperature dependences of $k_B^{-1}(F_{\text{Neel}} - F_{\text{Bloch}})$, where $F_{\text{Neel}}$ and $F_{\text{Bloch}}$ are the minimum free-energy of Neel state ($m_y=0$) and that of Bloch state ($m_z=0$), respectively. The value of $a$ is 0.8 nm and that of $l_z$ is 8 nm.

$l_z$ in experiment (2.5 nm) is smaller than 4 nm, the free-energy barrier of nano-contacts in experiment is considered to be smaller than 400 K, indicating that the magnetic structure of nano-contacts in experiment is thermally fluctuating at room temperature even without the Joule heating induced by the current conducting. Therefore, further study is required to clarify the effect of the thermal fluctuation of the magnetic structure to the MR signal. We also notice that the free-energy barrier vanishes around $l_x=20$ nm, indicating that the stable state changes there. The same change occurs at zero temperature at a similar value of $l_x/l_z$ [10].

4. Summary
We have investigated thermal stability of magnetic wall confined in a nano-contact by measuring free-energy as a function of magnetizations. To this end, we have developed an efficient Monte-Carlo method by combining the Stochastic Cutoff method [11] for long-range interacting systems with a variant of Wang-Landau method [12, 13]. We have found that nano-contacts with the ratio $l_x/l_z \approx 2.0$ are optimum as MR devices since the thermal fluctuation is inhibited due to their high-free-energy barrier and they show high MR signal due to their small radius.

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