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ABSTRACT
The influence of magnetic damages at the sidewall of perpendicular magnetic tunnel junctions (p-MTJs), which are the core devices of spin-transfer-torque magnetoresistive random-access memory (STT-MRAM), is discussed based on the thermal stability factor, \( \Delta \), double-logarithmic plot of normalized switching energy barrier, \( E \), and saturation magnetization, \( M_s \), and their exponential slope, \( n \). \( \Delta \) was calculated using the string method under the simulation conditions of domain wall motion switching. \( n \) increased with the increasing thickness of the damaged layer of the sidewall. Notably, the sidewall damage can be explained by the reduction in \( M_s \) and exchange stiffness constant, \( A_s \), rather than the interfacial perpendicular anisotropy. The findings of this study are important for controlling and improving the process damage in the mass production of p-MTJs in STT-MRAM.

I. INTRODUCTION
In the last decade, considerable effort has been dedicated to developing spintronics-based integrated circuits (ICs) with perpendicular magnetized magnetic tunnel junctions (p-MTJs) using interfacial perpendicular magnetic anisotropy (IPA) and \( \Delta \)-coherent tunneling technology.\(^7\) They offer high performance at low operation voltage, high endurance, and low power consumption owing to their non-volatile nature.\(^7\) Currently, spintronics-based ICs using spin-transfer-torque magnetoresistive random-access memories (STT-MRAMs) are about to enter into the mass production phase. With these features, spintronics-based ICs can be applied in a variety of applications, such as non-volatile microcontrollers.\(^7\) In general, STT-MRAM in ICs must operate in a specific temperature range, e.g., from \(-40^\circ C\) to \(150^\circ C\) for grade 1 of automotive application, and also it is necessary to withstand a temperature of \(260^\circ C\) when the reflow soldering process is used to attach chips to a printed circuit board.\(^8\) Hence, this means that it is important to understand how the performance metrics of the spintronics-based ICs vary with temperature. The thermal stability factor, \( \Delta = E/k_BT \), where \( E \) is the energy barrier, \( k_B \) is the Boltzmann constant, and \( T \) is the absolute temperature, is one of the most important performance
metrics as it determines the retention time of given bits in STT-MRAM. Because magnetic properties that determine $E$ in $\Delta$ are dependent on temperature, the manner by which $E$ scales with temperature should be elucidated. Generally, two different magnetization reversal modes dominate $E$, depending on the size of the $p$-MTJ: one is the domain wall propagation model, and the other is the coherent magnetization reversal model.\(^{14,15}\) However, $E$ cannot be experimentally explained\(^ {14,15}\), although the decrease in $E$ has been taken into consideration both domain wall propagation and coherent reversal model. Accordingly, the scaling down of $E$ in the experiment may be considered another effect, such as the damaged layer at the sidewall during the microfabrication process.\(^ {14,15}\)

If there is no detailed information on “what kind of damaged layer is formed,” IC design cannot be performed precisely. Detailed information on the damaged layer thickness and degradation of $M_s$, magnetic anisotropy, $A_s$, and $\Delta$ is difficult to understand using mere experimental data. Many reports are available on micromagnetic simulations because a simulation method can individually set damaged information.\(^ {16-18}\) A few studies have used the temperature dependence of $\Delta$ and magnetic properties of the damaged layer to reproduce experimental data. Thus, we think that it is important to deeply understand the temperature dependence of $\Delta$, including the damaged layer, to develop STT-MRAMs for industrial applications, such as automobiles and social infrastructure, where guaranteeing safety operation at high temperatures is required. In this study, a micromagnetic simulation based on the string method is used to calculate the temperature dependence of $\Delta$ using various types of magnetic parameters and reproduce the temperature dependence of $\Delta$ and magnetic properties in the experimental data of previously reported $p$-MTJs.\(^ {17}\)

II. THEORY

$\Delta$ and the switching mode of magnetization are strongly dependent on magnetic materials. High-crystalline magnetic anisotropy materials, such as $\text{La}_{2/3}$-ordered alloys, are attractive from the viewpoint of thermal stability with large $\Delta$. Because IPA in CoFeB/MgO can be compatible with Si-based CMOS technology, the magnetic properties used here for calculations refer to the CoFeB/MgO system. Here, the ideal temperature dependence of $E$ for $p$-MTJs with the CoFeB/MgO system based on the two-reversal models is described. The domain wall propagation model is observed at a large size of $p$-MTJs down to a critical $p$-MTJ size, below which the coherent magnetization reversal model is observed. For the domain wall propagation model, $E$ is expressed as $E = 4(A_s K_{\text{eff}})^{0.5} D t$, and for the coherent magnetization reversal model, $E = K_{\text{eff}} \pi (D/t)^2$, where $K_{\text{eff}}$ is the effective perpendicular magnetic anisotropy energy density, $t$ is the free layer thickness, and $D$ is the diameter of the circular $p$-MTJ. In these formulas, $A_s$ and $K_{\text{eff}}$ are the two relevant magnetic properties determining $E$. The temperature dependence of $A_s$ and $K_{\text{eff}}$ is correlated with that of $M_s$ through a power-law scaling relationship,

$$
\frac{A_s(T)}{A_s(T^*)} = \left( \frac{M_s(T)}{M_s(T^*)} \right)^2,
$$

(1)

$$
\frac{K_{\text{eff}}(T)}{K_{\text{eff}}(T^*)} = \left( \frac{M_s(T)}{M_s(T^*)} \right)^{-2},
$$

(2)

where $T^*$ is the normalizing temperature at 0 K. The power-law scaling for the temperature dependence of $A_s$ was reported in Ref. 20. $K_{\text{eff}}$ of the CoFeB/MgO system can be expressed as $K_{\text{eff}}(T) = K_i + \left( K_b - \frac{1}{3} M_b^2 \right) \frac{1}{T}$, where $K_i$ is the interfacial anisotropy at the CoFeB/MgO system, and $K_b$ is the bulk magnetic anisotropy energy density. Because the contribution of $K_b$ to $K_{\text{eff}}$ is negligibly small and the $T$ dependence of $K_i$ is correlated with that of $M_b$ through the power-law scaling with an exponent of approximately 2,\(^ {21,22}\) the exponent for the $T$ dependence of $K_{\text{eff}}$ should also be around 2. From these relationships, one can derive the following scaling relationships between the $T$ dependencies of $E$ and $M_s$, which is independent of the reversal model,

$$
\frac{E(T)}{E(T^*)} = \left( \frac{M_s(T)}{M_s(T^*)} \right)^{-2}.
$$

(3)

Although the value of the exponent is expected to be approximately 2, the experimentally determined value was much larger than 2 and ranged from 3 to 5.\(^ {17}\) One possible reason for the discrepancy can arise from the finite damage on the sidewall of the $p$-MTJ during device processing in the experiment.

III. METHODS

The energy barrier was calculated by the micromagnetic simulator EXAMAG\(^ {17}\) incorporating the string method. The string method\(^ {24-26}\) is useful in identifying the minimum energy path between the parallel ($P$) and antiparallel ($A$) states of MTJs. The magnetic energy states of the demagnetization energy for $z$ axis $E_{\text{dm}}$, anisotropy energy, $E_{\text{ani}}$, exchange energy, $E_{\text{exc}}$, and total energy, $E_{\text{all}}$, are calculated in each point in the free energy landscape between bistable states. $\hat{a}_1$ and $K_U$ are the unit vector of the magnetic easy axis and the uniaxial magnetocrystalline anisotropy constant, respectively. The energy states are described as follows:

$$
E_{\text{all}}(\hat{M}) = \frac{1}{2} \hat{M} \cdot \hat{H},
$$

(4)

$$
E_{\text{ani}}(\hat{M}) = \frac{K_U}{M_b^2} \left( \hat{a}_1 \cdot \hat{M} \right)^2,
$$

(5)

$$
E_{\text{exc}}(\hat{M}) = \frac{A_s}{M_b^2} \left( \left( \hat{\nabla} \cdot \hat{M} \right)^2 + \left( \hat{\nabla} \times \hat{M} \right)^2 \right),
$$

(6)

$$
E_{\text{all}} = \int dV \left( E_{\text{ani}} + E_{\text{exc}} + E_{\text{dm}} \right).
$$

(7)

A few studies investigated and calculated that $E$ and $\Delta$ have sidewall damages.\(^ {16}\) However, a full stacking structure is necessary in applications because such a structure can consider the influence of a stray field and exchange coupling in each layer.\(^ {27}\) Subsequently, the model of the stacking structure was a full stacking $p$-MTJ structure referenced from an experimental report\(^ {17}\) [Fig. 1(a)]. The junction diameter and the sidewall angle were 30 nm and 87.5°, respectively. The damaged layer was formed on the sidewall of the dot with a uniform thickness, and the diameter, including the damaged layer, was fixed at 30 nm [Fig. 1(b)]. The thickness of the damaged layer was 1 nm, 3 nm, 5 nm, and 7 nm. The magnetic parameters, $M_s$,\(^ {11}\) perpendicular magnetic anisotropy $H_{k_s}$, and $A_s$,\(^ {28}\) used in the calculation, were referred from the experimental results [Fig. 1(c)]. A
FIG. 1. (a) Stacking structure of $p$-MTJs, (b) junction diameter of 30 nm and damaged layer formed at the sidewall of the dot ($D = 1$ nm, 3 nm, 5 nm, and 7 nm), and (c) temperature dependence of magnetic parameters, $M_s$, $A_s$, and $H_k$, for simulation.

IV. SIMULATION RESULTS AND DISCUSSION

To reduce the total calculation cost, the magnetization curves ($M$–$H$) were simulated before the calculation of $E$, and we only calculated the minimum energy path from the P to AP state. Figure 2 shows the $M$–$H$ curves of the no-damage and 3-nm-thick damaged $p$-MTJs. $M_s$ and coercivity were decreased by the damage, and the amount of the reduction of coercivity depended on the type of damage. Figures 3(a) and 3(d)–3(f) show the magnetic parameters of $E_d$, $E_{ani}$, $E_{exc}$, and $E_{all}$ during the paths’ minimum motions between bistable states. The calculation is based on Eqs. (4)–(7). $\vec{H}$ is the static magnetic field vector, and $\vec{M}$ is the magnetization vector. $E_{all}$ can be described by the summation of each energy. The Zeeman energy was not included because the external magnetic field is not applied in the

part of these magnetic parameters were obtained from the film form, which is based on the fabrication process of an STT-MRAM on a 300 mm wafer. The decrease in $H_k$ was caused by the physical damage at the CoFeB/MgO interface. As such, the damages occurred during ion etching in the microfabrication process, and no change was found in the Curie temperature. The decrease in $M_s$ and $A_s$ may be caused by the inclusion of different atoms due to the chemical processes during microfabrication, and the Curie temperature was decreased. So, the process damage can be visualized by comparing the calculation and experimental results. Because $H_k$, $M_s$, and $A_s$ are related to one another in actual magnetic materials, the changes in $H_k$, $M_s$, and $A_s$ may not be completely independent. Therefore, the magnetic parameters in the calculation were utilized to stand out as possible as actual magnetic materials. Three different types of damage were assumed: (i) 50% of reduced $H_k$, (ii) 50% of reduced $H_k$ and 20% of reduced $M_s$ and $A_s$, and (iii) 50% of reduced $H_k$ and 40% of reduced $M_s$ and $A_s$. These magnetic parameters were set as the reference and recording layers. $A_s$ at the interface of the sidewall was set as the average of the damaged and no-damage values. The units used in this study are based on cgs.

FIG. 2. Normalized perpendicular magnetization ($M_z/M_s$) vs magnetic field ($H_z$) curves at 300 K for the $p$-MTJs with various damaged parameters.
FIG. 3. Demagnetization energy, \(E_d\), anisotropy energy, \(E_{ani}\), exchange energy, \(E_{exc}\), and total energy, \(E_{all}\) during the pathing minimum route for switching by the string method. [(a) and (d)] 5-nm-thick damaged layer with the magnetic parameters of 50\% of reduced \(H_k\) and 40\% of reduced \(M_s\) and \(A_s\) at 10 K and 450 K; [(b) and (c)] domain mapping of normalized perpendicular magnetization \((M_z/M_s)\) and \(E_{exc}\) corresponding to the damaged case described in Fig. 1(b); [(e) and (f)] no damaged dot at 10 K and 600 K.

Case of the string method. \(E_d\), \(E_{ani}\), and \(E_{exc}\) are the total energy of the full stacking of \(p\)-MTJs, and the corresponding domain images are the energies of each layer. The interlayer coupling of Ru also includes the curves of \(E_{exc}\). \(E_{exc}\) was at maximum at the antiparallel spin configuration and minimum in the parallel spin configuration, and these values are always positive due to the sign of \(A_s\). The vertical axis of the curves represents the energy, and the \(E_{exc}\) domain mappings are represented as erg/volume. Here, in the case of the \(E_{exc}\) curve, the sign of \(E_{exc}\) is negative because \(E_{exc}\) is the summation of the total layer. Figures 3(b) and 3(c) show the mapping images of the normalized magnetization, \(M_z/M_s\), and \(E_{exc}\) component, respectively. Each mapping image is presented as arrows in Fig. 3(a). \(M_z/M_s\) is aligned to the perpendicular direction in each bistable state. Figure 3(a) shows the results for the 5-nm-thick damaged layers with the damaged magnetic parameters of (iii) at 10 K. The cause of the asymmetric curve energy profiles is the influence of the stray field from the reference layer. \(E_{all}\), \(E_{exc}\), and \(E_{ani}\) show an upward convex curve, and \(E_d\) shows a downward convex curve. The domain images of \(M_z/M_s\) and \(E_{exc}\) showed the change in contrast during switching, which corresponds to the maximum point of \(E_{exc}\) in Fig. 3(a). These results indicate the formation of the domain wall during the energy path. The relative angle of magnetization increased with the formation of the domain wall at the saddle point. The \(M_z\) component decreased due to the relative angle of spins; therefore, \(E_d\) becomes the smallest when \(E_{exc}\) is the maximum. \(E_{all}\) decreased when the temperature increased to 450 K [Fig. 3(d)] due to the decrease in the base energy level \(E_d\), which indicates the decrease in the magnetostatics energy. In the case of \(E_{exc}\) at 450 K, the domain wall still exists at the saddle point. Figures 3(e) and 3(f) show the energy profiles at 10 K and 600 K for the \(p\)-MTJs without the damaged layer. The domain wall was also formed in the \(p\)-MTJs without the damaged layer. Although magnetic parameters are slightly different, the condition of the domain wall formation is almost consistent with that of previous results. Δ of the no-damage \(p\)-MTJs is higher than that of
the damaged $p$-MTJs. All the calculations in this study showed the domain wall motion, and a coherent switching was not observed.

Figure 4(a) shows the energy ($E$) and $\Delta (E/k_B T)$ for the 3-nm-thick damaged $p$-MTJs with damaged parameters of (i)–(iii). The $p$-MTJs without the damaged layer are used as control. The damaged $p$-MTJs show smaller $\Delta$ at all temperatures. The damaged parameters (ii) and (iii) were crossover at approximately 450 K, which is attributed to the temperature dependence of $H_k$ [Fig. 1(c)]. In order to estimate the slope with various types of damaged parameters, $E$ was systematically examined for the $p$-MTJs. Figures 4(a) and 4(b) show $E(T)/E(10 K)$ vs $M_s(T)/M_s(10 K)$ and (b) exponent value estimated from $E(T)/E(10 K)$ vs $M_s(T)/M_s(10 K)$. The thickness of the damaged layer was fixed to 3 nm. The exponent for the no-damage $p$-MTJs was approximately 2, which is consistent with that in Eq. (3). In the case of magnetic parameter (i), $H_k$ was reduced to half in the damaged layer. Here, $H_k$ is almost equal to $K_i$ because CoFeB is thin enough and perpendicular magnetic anisotropy (PMA) occurred at the interface between the CoFeB and MgO barriers. The exponent of 50% of $K_i$ was almost the same as that of the no-damage $p$-MTJs. On the contrary, when $M_s$ and $A_s$ were reduced to 80% with a $K_i$ of 50%, the exponent was increased. The exponent was increased to ~2.8 in the case of 60% of $M_s$ and $A_s$ and 50% of $K_i$. These results indicate that the magnetic parameters of $M_s$ and $A_s$ in the damaged layer clearly showed the differences in the exponent value.

To further understand the damage mechanism, various thicknesses of the damaged layers were systematically investigated. Figures 5(a) and 5(b) show various thicknesses and magnetic parameters for the damaged layer, and Fig. 5(c) shows their exponent. Note that the thicknesses, except 7 nm, had an exponent of approximately 2, with 50% of $K_i$ magnetic damaged parameter of case (ii). In the case of damage parameters (ii) and (iii), the exponent increased with the increase in the thickness of the damaged layer. By increasing the damaged layer to 7 nm, the magnetization switching was not a simple bistable state in the $M$-$H$ curves and magnetization switching through the mixture of perpendicular and in-plane magnetization. Therefore, the minimum energy paths are complicated, and $E$ cannot be decided in this work. Below the thickness of the damaged layer of 5 nm, $K_i$ did not show any differences in the exponent, but $M_s$ and $A_s$ showed evident defenses, and the decrease in these parameters influenced the exponent. Comparing the experimental data of $p$-MTJs (exponent $n = 3.1$), the simulation data of the 5-nm-thick damaged layer and the damage case of (iii) (exponent $n = 3.0$) showed almost consistent results. Hence, the type of damage in the experimental case is the impurity atoms that penetrated and diffused into CoFeB and degrade the magnetic parameters of $M_s$ and $A_s$, rather than the degradation of perpendicular magnetic anisotropy at the interface by physical damage. For the experimental data ($n = 3.1$), they used reactive ion etching and Ar ion milling as the patterning process for $p$-MTJs. Our
calculation was performed by considering the damage in the p-MTJ sidewall. Hence, the assumption is that the other atoms come from the outside of the p-MTJs, and the interdiffusion of each layer was considered. Thus, the process gases, such as nitrogen and hydrogen, used in the microfabrication degrade the magnetic properties of CoFeB. The management of process gases during microfabrication requires additional attention for preparing high-quality p-MTJs integrated to ICs.

V. CONCLUSIONS
The magnetization behavior of p-MTJs was calculated using the string method with various magnetic parameters and thicknesses of damaged layers. During the paths’ minimum energy motions, all the p-MTJs formed a domain wall during switching. Considering the double-logarithmic plot of the normalized switching $E_{(T)}$, $M_s$, and their exponent slopes $n$, $n$ was strongly influenced by the damage parameters of $M_s$ and $A_s$. The increase in $n$ in the experiment can be well explained by assuming that the impurities penetrate into the sidewall and formed a damaged layer. The magnetic stability of p-MTJs can be drastically improved by controlling the process gases during microfabrication.

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DATA AVAILABILITY
The data that support the findings of this study are available from the corresponding author upon reasonable request.

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