Cross-sectional Area Dependence of Tunnel Magnetoresistance, Thermal Stability and Critical Current Density in MTJ

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Tunnel magneto-resistance (TMR), thermal stability, and critical switching current are important metrics of a magnetic tunnel junction (MTJ). In this work, a detailed study of these metrics is conducted for the down-scaling of the transverse dimensions of the MTJ. The quantum transport and the magnetization dynamics simulations are performed using non-equilibrium Green's function in the mode-space approach and Object Oriented Micromagnetic Framework (OOMMF), respectively. The study of areal size quantization effects on the TMR shows that most of the contribution to the TMR comes from lower energy sub-bands and that the TMR saturates for dimensions above 50 nm. An anomalous behavior is observed in the bias dependence of TMR for the lower energy sub-bands and is explained in terms of the modified Slonczewski's analytical model for conductance around zero bias. The study of TMR scaling is extended to consider non-idealities by introducing elastic dephasing into our simulations. It is shown that with down-scaling of diameters, dephasing affects the zero bias TMR predominantly below 20 nm. Further, TMR is also studied in terms of sensitivity to the variations in the interface layer and the asymmetric reduction of TMR with bias and its reversal at higher bias is observed. OOMMF simulations of the larger stack, including the free layer, are carried out to understand the qualitative link between magnet switching behavior, thermal stability, and critical current density with area scaling. It is shown that the area dependence of thermal stability and critical current follow each other qualitatively and the scaling of both these metrics is correlated to different regimes of magnetization switching such as macrospin behavior or formation of metastable complex textures. The implications of scaling, on the various MTJ metrics, are discussed in terms of the application domain.

Index Terms— Critical current density, magnetic tunnel junction (MTJ), NEGF, quantization, TMR, and thermal stability.

I. INTRODUCTION

THE emerging non-volatile spin based memories, especially spin transfer torque random access memory (STT-RAM), are promising alternatives to memory devices, both in stand-alone configuration and embedding with CMOS for Non-Von Neumann computing [1]–[3]. Magnetic tunnel junction (MTJ) as the basic storage cell of STT-RAM, promises low power consumption, high endurance, fast switching performance and compatibility with CMOS due to non-volatility and efficient switching mechanisms such as spin transfer torque (STT) and spin orbit torque (SOT) [3]. Tunnel magneto-resistance (TMR), thermal stability (Δ), and critical switching current density (J_c) are important metrics of an MTJ with high device dimension dependence. TMR is expressed as $TMR = (R_{ap} - R_p)/R_p$, where R_{ap} and R_p are resistances of the MTJ in anti-parallel and parallel magnetization state. It determines the read margin, sense speed, and noise margin of a memory cell [4]. Hence, TMR is preferred to be high. Considering the quantization effects at lower dimensions, TMR is a strong function of both transverse dimensions of the entire device as well as the thickness of the tunnel barrier (TB). This is particularly true for Fe/MgO based systems due to the symmetry filtering property [5]. Quantization effects in the transverse plane result in a decrease

of TMR with an increase in dimensions, and normally around 50 nm, this value starts to saturate to a minimum [6], [7]. The other important metric used in MTJ performance characterization is its thermal stability which determines data retention, read disturbance, memory size, and operating temperature of the STT-RAM [4]. Stability (Δ) for dimensions below 30 nm can be approximated with Stoner-Wolfarth model as-

$$\Delta = \frac{E_b}{k_B T} = \left(-\delta N \frac{M_s^2}{2\mu_0} t + K_b t + K_i \right) \frac{\pi D^2}{4k_B T} \quad (1)$$

where E_b is the energy barrier between two stable states, k_B is the Boltzmann constant, and T is the absolute temperature, δN is the shape anisotropy coefficient, M_s is the saturation magnetization of free layer (FL), μ_0 is the permeability of free space, K_b is the bulk anisotropy energy density, K_i is the interface anisotropy energy density, D is the diameter of FL. But with an increasing cross-sectional area of the device, the mechanism of FL switching becomes complicated due to domain formation, making it difficult to have an empirical expression for Δ computation. The desired value of Δ depends upon the allowable chip failure rate and for practical applications it is expected to be greater than 60 [8], which has been difficult to achieve in nanomagnets that rely on bulk anisotropy. With the proper reduction of the thickness of the FL, the interface anisotropy term dominates resulting in

perpendicular magnetic anisotropy (PMA) MTJ with Δ increased above 60 [9]. However, with further scaling, i.e., with device transverse dimensions scaling below 20 nm, the PMA MTJ too has a limit and new method for achieving high Δ is utilizing shape anisotropy of MTJ by increasing thickness of FL beyond its lateral dimension so that the shape anisotropy itself results in PMA behavior [10]. Further, with increasing transverse dimensions Δ is expected to increase with a quadratic dependence on diameter up to macrospin approximation, beyond which it has been observed to increase as a linear or independent function of diameter [11], [12]. It should be noted that there are observations, both simulation and experimental [13], which deviate from the predicted behavior due to complex switching behaviors at higher dimensions. These include reverse domain nucleation and motion [14], the observed effect of scaling projections on Δ up to 100 nm diameters shows stability increasing much slower and change of switching mechanism from coherent taking more time to incoherent one, but not much qualitative reasoning has been provided [15]. The critical switching current is another important metric that determines the energy efficiency of MTJ and for low dimensions, the macrospin approximation can be employed to analytically predict the value but once the cross-sectional area increases, J_c behavior is affected by complex domain reversal switching mechanism. Further, Jaiswal also studied the effect of scaling on resistance-area (RA) product and critical switching current but this analysis is restricted to mono-domain approximation [16].

In this work, we have used the Non-equilibrium Green's function (NEGF) model to study the effect of quantization on the spin transport, reflected in TMR of the PMA-MTJ (CoFeB/MgO/CoFeB) device. Using the model in this manuscript we explain the contribution of different transverse modes to the experimentally observed TMR. Also, an anomalous behavior in lower sub-band TMR is observed and explained in terms of quantization effects and the results are benchmarked with the modified Slonczewski's model. The important guidance is that these results indicate that we will have to reduce the read bias regime with down scaling of cross-sectional dimensions. The effect of non-idealities on TMR with area scaling is also analyzed by including the dephasing into the model.

Further, micromagnetics based study is carried out for evaluation of metrics Δ and J_c , and their dependence on device cross sectional. A qualitative analysis of the effect of scaling on Δ and J_c for a range of diameters starting from 10 nm to 250 nm is provided. Combining all the results corresponding to TMR, stability, and critical switching current into one plot we conclude with the optimal lateral dimensions for various MTJ applications such as stochastic neuromorphic computing, MRAM, and large area sensors [17].

II. DEVICE MODELING

In this section, we provide the detailed methods used to model the spin transport and magnetization dynamics of the device. Fig. 1 shows the typical MTJ device structure considered in this paper. It is divided into two sub-structures: synthetic anti-ferromagnet (SAF) [FM1/Ru/FM2] responsible for the pinning of the pinned layer (PL) via a spacer (usually Tantalum (Ta)),

and MTJ active region (CoFeB/MgO/CoFeB). From the transport point of view, all MTJ action happens in the active region. Considering the role of quantization effects coming from lateral device dimensions, we first show the role of different transverse modes in TMR and its saturation with higher energy modes. The study of TMR area dependence is further carried out for a range of device lateral dimensions starting from 3 nm to 100 nm. To account for non-idealities, we introduce elastic dephasing into the device Hamiltonian to study dephasing effects at different values of cross-sectional areas. Micromagnetic simulations were later incorporated using Object Oriented Micromagnetic Framework (OOMMF), for the

Fig. 1. Magnetic tunnel junction device structure for NEGF and micromagnetic simulations.

active and SAF regions combined. These results allow us to propose a model based on multi-domain formation in the FL, particularly at larger cross-sectional areas. We also evaluate the Δ and J_c at different diameters, for both of these parameters we simulated the role of different regimes such as coherent and complex metastable texture-based magnetization reversal on Δ and J_c .

A. Spin transport with NEGF

The spin transport in MTJ is modeled by considering MgO as TB between two ferromagnets (FMs), PL (CoFeB), and FL (CoFeB) as shown in Fig. 1. Effective mass tight-binding (EMTB) model with the mode space approach [18] is used to represent the device Hamiltonian as shown in Fig. 2(a) and 2(b). The complete device Hamiltonian is expressed as-

$$H_D = H_{LFM} + H_{I1} + H_{TB} + H_{I2} + H_{RFM} \quad (2)$$

where, H_D is the complete device Hamiltonian consisting of the H_{LFM} , H_I , H_{TB} , H_{RFM} corresponding to the Hamiltonians of left FM, interface, TB, and right FM respectively. Assuming a coherent interface between FM and TB ensures that momentum parallel to interface (x , y) is conserved. This allows us to decompose the device Hamiltonian into transverse and longitudinal (z) parts, thus we invoke mode space approach to compute spin and charge current by considering each transverse mode as a 1D independent transport channel. Now, considering periodicity in the x - y plane, we describe the 2D effective mass

Hamiltonian for both FM layers and TB in terms of onsite potential ε_0 , and hopping parameter t is given by-

$$t = \frac{-\hbar^2}{2ma^2} \quad (3)$$

Where, $\hbar$, m , and a are reduced Planck's constant, effective mass of electron in respective material and lattice spacing in the

Fig. 2 (a). Representation of tight binding model used for active region, **(b)** 1D lattice sites in transport direction representing the Hamiltonian of 1 mode.

model, respectively. We devise the H_T for both FMs and TB separately. In 2D we define our Hamiltonian as shown in Fig. 2 (a), which is described as-

$$H_T(i, j) = \begin{cases} [h_{00}], & \text{when } i = j \\ [-h_{10}], & \text{when } i = (j - 1) \\ [-h_{01}], & \text{when } i = (j + 1) \\ [Z], & \text{otherwise} \end{cases} \quad (4)$$

Here we have considered the nearest neighbor interactions only. h_{00} , h_{01} , h_{10} are the Hamiltonian matrices corresponding to the 1D chain of unit cells in z direction and Z is the matrix of zeros.

$$h_{00}(k, n) = \begin{cases} \varepsilon_0 + 4t, & \text{when } k = n \\ -t, & \text{when } k = (n - 1) \\ -t, & \text{when } k = (n + 1) \\ 0, & \text{otherwise} \end{cases} \quad (5)$$

Here, k and n correspond to unit cells in x direction, $(\varepsilon_0 + 4t)$ is the onsite energy, $-t$ models the hopping of an electron from k to $k-1$ and $k+1$.

$$h_{01}(k, n) = \begin{cases} -t, & \text{when } k = n \\ 0, & \text{otherwise} \end{cases}, h_{10} = h_{01}^+ \quad (6)$$

We compute the respective eigen states of H_T which act as transverse modes, thus conduction band minima for our computation of different charges and spin currents.

The longitudinal Hamiltonian as a chain of 1D lattice site shown in Fig. 2 (b) is defined as

$$H_L(i, j) = \begin{cases} \varepsilon_c + 2t, & \text{when } i = j \\ -t, & \text{when } i = (j - 1) \\ -t, & \text{when } i = (j + 1) \\ 0, & \text{otherwise} \end{cases} \quad (7)$$

where ε_c is the conduction band minima which we computed from H_T . So, for each ε_c , we have the same H_L which is subsequently used in NEGF to compute currents and other transport properties. Here, t differs according to the material. So, for FM we have

$$t_{fm} = \frac{-\hbar^2}{2m_{fm}a_{fm}^2} \quad (8a)$$

$$\text{while for MgO} \quad t_{ox} = \frac{-\hbar^2}{2m_{ox}a_{ox}^2} \quad (8b)$$

For these simulations, we used CoFeB as FM. Therefore, $m_{fm} = 0.8*m_e$ and $a_{fm} = 2.89 \text{ \AA}$. For MgO, m_{ox} lies between $0.18*m_e$ to $0.3*m_e$ and $a_{ox} = 4.05 \text{ \AA}$. The onsite potential at each site in terms of barrier height above fermi-level U_b (eV), exchange splitting in FMs Δ_{ex} (eV) along with the external voltage V (V) drop across MgO (assuming zero resistance of FMs and other layers compared to the barrier) is modeled as-

$$U_{onsite} = \begin{cases} U_b \delta_{i,j} I_{2 \times 2} & i, j \text{ are the indices of Hamiltonian corresponding to MgO} \\ \frac{(I_{2 \times 2} - \vec{\sigma} \cdot \vec{M}) \Delta_{ex}}{2}, & \text{for pinned layer CoFeB} \\ \frac{(I_{2 \times 2} - \vec{\sigma} \cdot \vec{m}) \Delta_{ex}}{2}, & \text{for free layer CoFeB} \end{cases} \quad (9)$$

$$U_{applied}(i, i) = \begin{cases} \frac{-qV}{2}, & 1 \leq i \leq N_{FL} \\ -qV \left[\frac{1}{2} - \frac{i}{N_o} \right], & 0 \leq i \leq N_o \\ \frac{-qV}{2}, & N_o + 1 \leq i \leq N_p \end{cases} \quad (10)$$

The complete device Hamiltonian corresponding to each transverse mode is-

$$H = H_T + U_{onsite} + U_{applied} \quad (11)$$

Further, all our calculations have to include the spin information corresponding to up and down spins, so, each site is represented by a 2×2 matrix. We compute the self-energy matrices describing the coupling of semi-infinite contacts (reservoirs) with the device as

$$\Sigma_{L,R} = \begin{bmatrix} -t_f \exp(ik_{\uparrow(L,R)} a_f) & 0 \\ 0 & -t_f \exp(ik_{\downarrow(L,R)} a_f) \end{bmatrix} \quad (12)$$

where $k_{\uparrow}$ and $k_{\downarrow}$ are momentum wave vector for up and down spin respectively, computed from the band structure (E, k) through tight-binding formalism. Here, assuming some portion of FM as contact and some as part of the device. The retarded Green's function describing this device is computed as per [19]

$$G^R(E) = [(E + i\eta) - H - \Sigma_L - \Sigma_R]^{-1} \quad (13a)$$

And advanced Green's function as

$$G^A(E) = G^R(E)^+ \quad (13b)$$

Where E is the energy range of interest in the transport direction.

Solving it further the current between unit cell k and $k+1$ is computed by

$$I_{C\sigma} = \text{trace} \left\{ \Sigma_{k_t} C_{\sigma} \frac{i}{\hbar} \left\{ H_{k,k+1} G_{k+1,k}^n - G_{k,k+1}^n H_{k+1,k} \right\} \right\} \quad (14a)$$

Resistance in the parallel (P) and anti-parallel (AP) states is simply computed from the expression-

$$R_{p,ap} = \frac{V}{I_{p,ap}} \quad (14b)$$

Thus, TMR is given by $TMR = \frac{R_{ap}-R_p}{R_p}$

Where $I_{p,ap}$ is the current carried by MTJ in P and AP state.

B. Micromagnetics

In this section, we present the methodology adopted for the study of J_c and Δ dependence on device cross-sectional dimensions. Here, we consider a PMA-MTJ with a circular cross-section, as shown in Fig. 3. The PL magnetization is pinned in a certain direction by exchange bias from SAF. We used the micromagnetic simulator OOMMF [20] that is based on the Landau–Lifshitz–Gilbert (LLG) equation and included the Slonczewski's STT extension module [21] to observe the STT magnetization switching of FL in the presence of spin polarized current.

The LLG equation encompasses the details of various forces acting on a magnetic moment in terms of different torques as below and provides the temporal evolution of net magnetization [22].

$$\frac{dm}{dt} = \frac{-\gamma}{1+\alpha^2} \left([m \times H_{eff}] + \alpha \times [m \times (m \times H_{eff})] \right) - a_{STT} m \times (m \times M) - b_{STT} m \times M \quad (15)$$

Where, m and M are the normalized unit vector magnetization of FL and PL, respectively. H_{eff} is the effective magnetic field given by

$$H_{eff} = H_{ext} + H_{exc} + H_k + H_d + H_A \quad (16)$$

where, H_{ext} , H_{exc} , H_k , H_d , and H_A are the external, exchange, anisotropy, demagnetization, and oersted fields, respectively.

The spin torque terms added to LLG are Slonczewski (in-plane) torque and field torque respectively. The former has anti-damping nature hence, is mostly responsible for switching [23].

$$a_{STT} = P \frac{h}{2e\mu_0 M_s t_{fm}} J \quad (17)$$

P is the polarization or spin torque efficiency coefficient ($P=0.7$).

$$b_{STT} = (b_0 + b_1 J + b_2 J^2) \quad (18)$$

Here, b_0 , b_1 and b_2 are *zeroth*, *first* and *second* order perpendicular components of spin transfer torque, b_0 is equilibrium IEC between PL and FL, respectively. Here, $b_1 = 2.7 \times 10^{-9}$ m and $b_2 = 2.8 \times 10^{-19}$ m³/A.

It should be noted that the effective field is given by

$$H_{eff} = -\frac{1}{\mu_0 M_s} \frac{d\xi}{dm} \quad (19)$$

where ξ is the local magnetic energy density.

For the study of stability Δ and J_c , we have assumed the circular cross-sectional geometry discretized into cubic cells of $1 \text{ nm} \times 1 \text{ nm} \times 1 \text{ nm}$. We start our analysis with an MTJ with varying diameter from 10 nm to 160 nm . The staircase demag artifact which becomes prominent for the cubic meshes and effects has been reduced by introducing the *EdgeAnisotropy* K1. Here, we used the OOMMF package to find out minimum energy paths MEP corresponding to AP-to-P and P-to-AP switching, respectively. The stability is directly computed by

taking the energy barrier between two stable states corresponding to the MEP. To compute the J_c we took 1000 stages for simulation which correspond to 10 ns simulation time. This value was chosen by considering that any switching time above 10 ns reduces the device applicability in terms of speed.

C. Simulation details and parameter values

The parameters considered for quantum transport simulations, such as Fermi energy level (E_f), barrier height (U_b), exchange splitting in CoFeB (Δ_{ex}), effective mass of an electron in CoFeB (m_{fm}) and MgO (m_{ox}), and lattice parameters were adopted from [24] and are given in table I. Similarly, the parameters and constants for micromagnetic simulation followed in this work including saturation magnetization (M_s), thickness for different FM layers along with other parameters are given in Table II. The pinning is ensured by giving an external bias field of 5 kOe to the bottom layer and keeping uniaxial anisotropy of the bottom layer and pinning magnet higher than the free layer. This results in the strong pinning of the free layer. We note that dependence check on each parameter was performed to obtain optimized values of parameters provided in Table II. These values are consistent with the parameter range provided in [25, 26, 27]. Also, OOMMF simulations were carried out at 0K and field torque was neglected.

TABLE I

E_f (eV)	U_b (eV)	m_{fm}	m_{ox}	Δ_{ex} (eV)
2.25	0.9-1.1	$0.8m_0$	$0.22m_0$	2.11

TABLE II

Material	Saturation Magnetisation (A/m)	Exchange Stiffness Constant (J/m)	Inter Layer Exchange Coupling (IEC) (J/m ²)	Uniaxial Anisotropy (J/m ³)	Thickness (nm)
CoFeB (FL)	1.1E+06	1.3E-11	-	1.2E+05	2
MgO	-	-	-	-	1
CoFeB (PL)	1.3E+06	1.3E-11	-	5E+05	2
Ta	-	-	-3.8E-03	-	1
(CoPt)n	1.3E+06	1.3E-11	-	4E+05	-

III. RESULTS AND DISCUSSIONS

A. TMR

We study the role of the area on the TMR of an MTJ by resolving the current transport mechanism into different transverse modes. In Fig. 3 (c) we show TMR for each group of 100 modes in ascending order of energy starting from 1 till 900 modes of a $40 \text{ nm} \times 40 \text{ nm}$ device. TMR for higher energy modes increases sharply because the polarization of FM increases for higher energy transverse sub-bands as shown in Fig. 4. But, TMR computed for all 900 modes together is less than the average of the whole group, which is justified by the fact that individual TMR for higher modes is high but the current carried by these modes is very low compared to lower energy modes. So, the effective TMR finally saturates to some value below the average of all modes as shown in Fig. 3 (c). In

Fig. 3. (a) Transmission as function of E_z at increasing transverse energies, clearly $T(E_z)$ for lowest sub-bands is large. (b) Current and TMR for different transverse mode. (c) Transverse Sub-band energy versus TMR. Note that the Transmission and TMR in (a) and (b) were computed at read bias of 0.1 V

Fig. 3 (b) we observe that current for lower transverse energy sub-bands is quite high compared to the higher sub-bands. Thus, most of the contribution in experimentally observed TMR comes from lower sub-bands. The effective TMR found in experiments and simulations can be expressed as

$$TMR_{(observed)} = \frac{\sum_i (TMR_i \times I_{APi})}{\sum_i I_{APi}} \quad (20)$$

Here I_{APi} and TMR_i are the transverse energy resolved AP current and TMR corresponding to i^{th} range of sub-bands taken into consideration. In Fig. 3(c) we also observe that higher transverse sub-band TMR rolls down quite sharply away from zero bias compared to lower sub-band TMR. Normally, experiments show a TMR- bias trend somewhat between the higher and lower sub-bands. The simulations show an increasing trend of TMR with bias in a certain symmetric bias regime around the zero bias particularly, for lower sub-bands the bias range for this increasing behavior is large and it decreases while moving up in the higher energy transverse sub-band. This anomalous lower sub-band TMR obtained from NEGF simulation, can also be explained analytically by using

the modified version of Slonczewski's model for conductance at zero bias [28]. The effective polarization of each FM/TB interface is given by

$$P(E, V = 0) = \left(\frac{k_{\uparrow} - k_{\downarrow}}{k_{\uparrow} + k_{\downarrow}} \right) \left(\frac{k^2 - k_{\uparrow} k_{\downarrow}}{k^2 + k_{\uparrow} k_{\downarrow}} \right) \quad (21)$$

We introduced the effect of external bias in Eq. 21 by using WKB approximation [29] inside barrier to get the different wave vectors in terms of longitudinal energy, exchange splitting, barrier height and external bias for different transverse sub-bands as

Where, $k_{\uparrow, \downarrow}$ is the wave vector for spin up and spin down electron inside the FM while k is the wave vector inside the TB.

Fig. 4. Effective polarization as function of bias at various sub-band energies. Clearly, we can observe polarization at lower sub-bands is first increasing symmetrically around read bias regime then decreasing but on increasing transverse energy the increasing TMR-bias range keeps on decreasing.

$$P_{LF}(E_x, V, E_t) = \left(\frac{\left(\frac{\sqrt{E_x - E_t + V/2 + \Delta_{ex}}}{\sqrt{E_x - E_t + V/2 - \Delta_{ex}}} - \left(\frac{\sqrt{E_x - E_t + V/2 + \Delta_{ex}}}{\sqrt{E_x - E_t + V/2 - \Delta_{ex}}} \right) \right)}{\left(\frac{\sqrt{E_x - E_t + V/2 + \Delta_{ex}}}{\sqrt{E_x - E_t + V/2 - \Delta_{ex}}} + \left(\frac{\sqrt{E_x - E_t + V/2 + \Delta_{ex}}}{\sqrt{E_x - E_t + V/2 - \Delta_{ex}}} \right) \right)} \right) \left(\frac{(U_b + E_t - V/2 - E_x) - \left(\sqrt{E_x + V/2 - E_t}^2 - \Delta_{ex}^2 \right)}{(U_b + E_t - V/2 - E_x) + \left(\sqrt{E_x + V/2 - E_t}^2 - \Delta_{ex}^2 \right)} \right) \quad (22)$$

Here, P_{LF} , E_x , E_t , U_b , V and Δ_{ex} are effective polarization of left FM, longitudinal (transport) direction energy, transverse sub-band energy, TB height, external bias, and exchange splitting in left FM, respectively. Similarly, the effective polarization of right FM is computed as P_{RF} . The TMR in terms of polarization is given by

$$TMR = \frac{P_{LF} P_{RF}}{1 - P_{LF} P_{RF}} \quad (23)$$

We simulated the bias dependence of the effective polarization product of the structure at various transverse sub-band energies as shown in Fig. 4. It is observed that for lower sub-bands, the product of the left and the right polarization increases with bias for a certain symmetric range across zero bias, thus TMR increases during this period as computed by our NEGF model. Beyond a certain maximum, we see the decreasing trend of $P_{LF} \times P_{RF}$. Likewise, TMR starts rolling

with bias. However, for increasing transverse energy, the increasing TMR-bias range keeps on decreasing and at a certain value of transverse energy, the polarization attains global maxima at zero bias normally found in experimental results. It can be predicted from these results that for large-area devices since transverse sub-bands come much closer to each other and transport is restricted to lower sub-bands only, we may expect this sort of TMR behavior in large-area devices.

Further, we note that the observed TMR-bias dependence is normally a smoothly decreasing function with global maximum only at zero bias, which we also observe when taking the weighted sum of individual energy resolved TMR using (20). Further, while evaluating the TMR-area dependence as shown in Fig. 6, we studied the TMR for diameters varying from 3 nm to 100 nm. We observed an increasing trend of TMR with lower cross-sectional dimensions of MTJ with some fluctuations below 16 nm. Particularly, for 7 nm and 16 nm, the simulation results show bit higher values of TMR, deviating from previous results of monotonic decrease as explained by [7]. The TMR starts to saturate at a lower value for diameter around 40 nm, which can be considered as the diameter of a mono-domain FL. Here, the observed unusual behavior in TMR area dependence for 7 nm and 16 nm is expected to be coming from the fact that TMR depends upon the energy levels of different sub-bands with respect to lowest transverse energy. The sub-bands in lower cross-section area devices are separated further in energy. Thus, for 7 nm and 16 nm, the distribution of transverse sub-bands results in unusual TMR. The important point to note from these results is that we will have to reduce the read bias regime with down-scaling of area. For lower dimensions more of the higher energy sub-bands will start dominating the overall contribution in TMR, resulting in a sharp decrease of TMR with bias.

To include the non-idealities into our simulation we introduced the dephasing into device Hamiltonian in terms of modified total self-energy matrices as

$$\sum_{d \text{ in}} (E) = D \otimes G(E) \quad (24a)$$

$$\sum_d (E) = D \otimes G^n(E) \quad (24b)$$

Here, dephasing coefficient matrix (D) is chosen according to nature of dephasing for momentum relaxation type $D=D_0\delta_{ij}$ [30], specifying the correlation between the neighboring random atomic potential at the site ' i ' and ' j ' $D_{ij} \propto \langle U_i U_j^* \rangle$, while $G(E)$ is the Green's function and $G^n(E)$ is the electron correlation function. The effect of magnitude of dephasing at a fixed diameter has been studied by [6]. We further extend these studies to analyze the effect of dephasing with scaling of MTJ cross-sectional dimensions. For the range of diameters from 3 nm to 60 nm, we study the effect of dephasing on these different devices. Here, we observe that the dephasing largely affects the TMR corresponding to lower diameters and this behavior starts saturating after 40 nm. This is attributed to the introduction of extra spin independent energy levels near lower transverse sub-band energies. For lower diameters, the transverse energy quantization gap is large. So, these scattering energy levels reduce the difference of current carried by up spin and down spin ($I_{up} - I_{dn}$) which reflects as reduced TMR. For large

Fig. 5. (a) Effect of elastic dephasing on TMR with area scaling, here the magnitude of dephasing constant is varied from 0 to 2.6 eV² around zero bias. We observe dominant effect of dephasing for lower size MTJs in terms of TMR lowering, while dephasing has small and saturating effect for large MTJs. (b) Effect of dephasing magnitude on TMR size as parameter. Indicating dominance of dephasing on small size MTJs. (c) TMR Interface sensitivity of TMR, the asymmetric roll of the TMR with bias and its reversal around -0.5 V indicates the surface resonance which increases the conductance for both up and down channels for negative bias regime, thus reducing the effective TMR.

diameters, because of large number of sub-bands, these scattering energy levels cannot dominate. Thus, while down-scaling the lateral dimensions of MTJ device, we predict that dephasing will be a challenge. For higher diameters we can see that the TMR is gradually saturating to a minimum, because for same transverse cut off ratio of numbers of up and down

channels remains same but difference in net current carried by these channels in P and AP states is reduced which limits the TMR to a saturating value also shown in [6] [7]. Further, to study the effect of TMR sensitivity on interface quality in terms of disorder such as roughness and bonding at the interface, we varied the onsite potential corresponding to interface layer atoms, and asymmetric variation of TMR is observed. The Hamiltonian for the scattering region of the device becomes

$$H = H_{LFM} + H_{I1''} + H_{B'} + H_{I2''} + H_{RFM} \quad (25)$$

Here, $H_{I''}$ is the modified interface Hamiltonian with random disorder potential. Degree of asymmetry depending upon onsite energy which itself depends upon coupling of interface site with electrode [31]. The results in Fig. 5(c) depicts the asymmetric lowering of TMR and its reversal at -0.5 V for 12% variation (lowering) of onsite potential. In our simulations, the onsite potential for the interface is computed as a weighted average of CoFeB (FM) and MgO (TB)

$$\varepsilon_{on(I_f)} = \frac{x\varepsilon_{on(FM)} + y\varepsilon_{on(MgO)}}{x+y} \quad (26)$$

Here $\varepsilon_{on(I_f)}$, $\varepsilon_{on(FM)}$, and $\varepsilon_{on(MgO)}$ correspond to the onsite potential of interface, FM, and MgO respectively, while x and y are weights corresponding to FM and TB. The behavior of asymmetric TMR and its reversal is a characteristic of surface resonant states being formed that can be due to intentional doping by carbon or boron or some other interface disorder such as roughness [25]. The interface resonance increases the conductance for both types of spins hence reducing Δ band filtering property of MgO which reduces TMR [32] and at higher bias, the conductance of AP state increases more than P state. Thus reversal of TMR is possible as observed by [33].

B. Thermal stability and critical current density

Fig. 6. The snap shots of the PMA-MTJ (diameter 10 nm) magnetization configuration of the free layer showing coherent single domain switching.

The FL magnetization switching mechanism affects area dependence of J_c and Δ . As shown in Fig. 6 and 7, for the MTJ of 10 nm diameter, we observed that the time evolution in Fig. 6 of the spin configuration of FL follow the coherent switching process as a mono-domain, suitable for the macro-spin model approximation. But with the increasing area, exchange length starts playing a vital role to create a characteristic spin

configuration. The exchange length is the function of exchange stiffness and effective anisotropy including magnetostatic energy, which governs the width of the transition between magnetic domains. As seen in Fig. 7 for the diameter of 160 nm, the switching starts with creation of symmetric metastable textures, which increase their size with switching time. Interestingly, a symmetry between the magnetization of textures is retained till approximately 50% time of the switching.

Till 40 nm diameters, coherent switching takes place. As the size of the FL increases further, formation of complex metastable domains begins and the incoherent switching of free layer magnetization take place. An increased area of the switching layer easily forms complex spin texture as shown in Fig. 7. The formation of these metastable complex domains with area increase is one of the main factors to the rising and

Fig. 7. The snap shots of the PMA-MTJ (diameter 160 nm) magnetization configuration of the free layer different instant of switching. The symmetry in textures can be observed until half the switching period

eventual saturation in switching current density. The analytical expression for switching current density is given by [34]

$$J_c = \frac{\alpha}{b} \left[H_{eff} + \frac{1}{2} (N_y + N_z - 2N_x) M_s + \frac{2A_{ex}}{\mu_0 M_s} k^2 \right] \quad (27)$$

where, N_x , N_y , and N_z are demagnetization coefficients for thin-film FL, we have $N_z=1$, $N_x = N_y = 0$, H_{eff} is the effective field including fields like STT term, stray and Oersted fields, α is Gilbert damping constant, t_f is the thickness of FL, μ_0 is the permeability of free space, and b is given below

$$b = P \frac{\hbar}{2e\mu_0 M_s t_f} \quad (28)$$

where P is the spin polarization of PL. The second term in (27) corresponds to the demagnetization field. Since the larger junction can reduce demagnetization energy more easily by forming complicated spin configurations as shown in Fig. 7. Its effect can be observed in both J_c plot with the area and Δ versus area. In Fig. 9 after 75 nm diameter both J_c and Δ scale gradually with area. The last term in (27) describes the role of exchange stiffness A_{ex} and k . Here, k is the magnon wave vector

which gets quantized with the diameter, k is zero for the macrospin model, and for certain diameters, we observe Δ to be

Fig. 8 (a)–(b) minimum energy path taken by free layer magnetization while switching, from this we get energy of free layer while switching.

increasing till 75 nm indicating some role of stability increase due to k .

B.1. Dependence of thermal stability and critical current density on the cross sectional area of MTJ device
The thermal stability (Δ) of MTJ is a decisive metric for data retention capability, operating temperature, read disturbance, and memory size of the device. There have been several reports on thermal stability and critical current density. The experiments show that thermal stability shows a saturating behavior post critical diameter ~25 nm [35], ~44 nm [36]. But, reports such as [37] have shown increasing trend from 5nm onwards. More importantly the following reports [38] and [39] have shown both stable and increasing behavior of thermal stability with increasing diameter from 50 nm to 100 nm respectively. The saturating behavior is observed while using macrospin approximation-based fitting while the increasing trend is observed for domain wall fit. Since our discussion has also considered macrospin below 50 nm while metastable domains above 50 nm we consider [38] and [39] as a benchmark to validate our micromagnetic simulations.

The main objective while studying the scaling of thermal stability and critical current density with area was to understand

the qualitative link between switching behavior, thermal stability and critically current density for various diameters

The Δ is decided by the energy barrier between two stable states of FL magnetization as shown in Fig. 8. For diameters below 30 nm, we can observe that the FL is switching coherently as a monodomain, as shown in Fig. 8(a). We use a macrospin model which analytically predicts the Δ by

$$\Delta = \frac{E_b}{k_B T} \quad (29)$$

Here,

Fig. 9 (a) MTJ Critical switching current density versus diameter **(b)** Thermal stability versus diameter. Clearly, it can be observed that thermal stability and critical current density follow the macrospin model for lower diameters but this model fails to capture complex domain reversal-based switching at higher diameters.

$$E_b = \left(-\delta_N \frac{M_s^2}{2\mu_0} t + K_b t + K_i \right) \frac{\pi D^2}{4k_B T} \quad (30)$$

where, δ_N and D are the demagnetization coefficient for the thin-film magnetic layer (~1) and its diameter, respectively.

But, once the diameter is increased above exchange length we observe that magnetization switching becomes complex with metastable domain like texture based-reversal dominating the switching process. With further increase of diameter, switching occurs through multi-domain formation Fig. 8(b). Thus, it becomes difficult to analytically compute Δ of MTJ. Certain work [40] have come up with approximate analytical expressions for domain reversal based switching. But, these may not work for current induced switching as these are based on field switching. Also, they have considered few diameters

so, not applicable at higher diameters. We evaluate Δ for diameters starting from 10 nm up to 160 nm as shown in the Fig. 9, for diameters below 30 nm we observe some linear dependence of Δ on diameter, which is also expected by the fact that at lower cross sectional dimensions interfacial anisotropy reaches a physical limit while achieving reasonable Δ [9]. As we increase the diameter above 20 nm, we begin to observe the quadratic increase in Δ which fits the macrospin approximation as expected and this behavior is observed till 50 nm. Increasing diameter above 50 nm we observe Δ increasing gradually due to complex metastable domain formation and switching overtakes the coherent one hence decreasing Δ of the FL. The behavior of stability versus area curve is somewhat qualitatively matching critical current versus area curve, which is expected as the critical current density for switching is determined by the stability of domain as explained earlier. It is to be noted that the mutual dependence of various parameters complicates the experimental study of P-MTJ, which only could be revealed by micromagnetic studies, which is beyond the scope of the present study. We performed various parameter dependence check in order to obtain optimized parameters for reducing J_c in our simulations, as reported in (Fig. 7 to Fig. 10) respectively. Since different experimental reports show contradicting results corresponding to these metrics, we have focused on both simulation and experimental reports that validate that our simulation results lie in a reasonable and expected range.

Fig.10. TMR, critical current density and thermal stability dependence categorized into three regions according to MTJ device applications. Here region (a), (b) and (c) correspond to special stochastic neuromorphic computing (Probability bits), Embedded and standalone MRAM and large application magnetic sensors respectively. The inset provides more details about the TMR below 10 nm.

In Fig. 10, the area dependence of the TMR, thermal stability, and critical current density is put together into a single plot, categorized into three regions suggesting optimum range for different MTJ applications, such as lower diameter MTJ devices are suitable for the special stochastic neuromorphic computing such as Probability bits (p-bits) and random number generators due to the high TMR but low thermal stability making them highly temperature-dependent at the same time switching current is also low [41]. The diameters between 30 nm and 80 nm are best suited for embedded MRAM as TMR is

good enough for this application, while thermal stability above 70 ensures data can retain for many years [42]. MTJ with a diameter above 80 nm can be utilized as large-area magnetic sensors. As the thermal stability corresponding to these diameters is above 100, which ensures these devices can sustain very high temperatures while maintaining non-volatility, these can find applications in non-destructive testing systems used for detecting small defects in conductive materials [43].

IV. CONCLUSION

Non-equilibrium Green's function and the OOMMF package were used to model the spin transport and magnetization dynamics, respectively, of an MTJ to understand its scaling behavior. The coherent nature of spin transport enabled us to use the mode space approach for resolving the terminal quantities in terms of underlying transverse modes. We observe that the TMR generally reduces from 5nm to 50 nm, displaying anomalous behavior at some dimensions. This behavior is explained in terms of the contribution of different conducting sub-bands to the TMR. The analysis of TMR in the presence of dephasing at varying diameters and bias indicates that dephasing affects the TMR significantly around the read bias regime below a few tens of nanometer diameter. Interface disorder affect an asymmetric lowering of TMR and finally its reversal at large bias.

From the magnetization dynamics perspective, the thermal stability and critical current density versus area were simulated and found initially increasing as per the macro-spin model. Then, both the metrics begin to evolve according to the complex domain reversal found in larger magnets. For such cases, the macro-spin model needs to be replaced by the domain wall model and the switching behavior can be understood in terms of exchange length and domain wall quantization effects. The behaviors of thermal stability and critical current density were observed to qualitatively match each other as a function of the MTJ cross-sectional area.

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