Superlattice-barrier magnetic tunnel junctions with half-metallic magnets

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Abstract
Spin-transfer torque (STT) applications in magnetization switching such as magnetic tunnel junctions (MTJs) have been of popular interest in the development of novel memory technologies. However, the high switching power associated with these is a critical disadvantage in the operation of typical magnesium oxide (MgO)-based STT-MTJs. In this study, an ultra-low switching power, only 10% of the MgO-based MTJs, is achieved by high-purity spin polarization current using a superlattice-barrier MTJ with half-metallic magnets. The resistance-area product of the device is reduced to $0.2 \ \Omega \ \mu m^2$, which is less than 10% of that in traditional MgO-based MTJs. The proposed MTJ has a higher performance, including STT and required switching current. A decrease in the switching power could avoid not only the disadvantages of power dissipation but also the device endurance due to lower Joule heating in the proposed MTJs.

1. Introduction
Emerging cutting-edge applications of the physical mechanism, spintronics, have become very important in overcoming the limitations of traditional memory technologies. Magnetoresistance (MR) effect provides a new concept of spin operation via magnetic tunnel junctions (MTJs) [1, 2]. MTJs with a magnesium oxide (MgO) tunneling barrier show strong tunnel magnetoresistance to realize the possibility of novel data storage and other spintronics devices [3–6]. Subsequently, the advent of the spin-transfer torque (STT) effect [7–9] in magnetoresistive random access memory (MRAM) exhibits some characteristics, such as non-volatility, high integration, and almost zero standby power consumption, in applications of MgO [9–12], which were never observed in traditional non-magnetic (NM) systems. However, the MgO barrier generally results in a large resistance-area (RA) product in MTJs. In MgO-based STT-MTJs, the writing mode requires a larger amount of power because the current passes the MgO tunneling barrier with a high RA product. Hence, the disadvantages of excessive switching power and insufficient spin-torque efficiency are major obstacles to the development of STT-devices. The restriction of the MgO barrier maintains an RA product higher than $7.0 \ \Omega \ \mu m^2$ [9, 13]. Large RA products produce a rapid enhancement of power consumption due to the increased write efficiency. These are sticky issues with the thermal regime for Joule heating, leading to the degradation of the MgO [14–16].

A multilayer structure in the barrier region has been studied for STT-MTJs to improve the disadvantage of the MgO barrier. Owing to its unique resonance properties, the double-barrier (DB) with F/I/N/I/F structure has shown a higher MR ratio and STT than the single MgO barrier MTJ [8]. Moreover, a superlattice-barrier (SLB), also called as the metamaterial or artificial material, is used to replace the high-quality MgO (100) tunnel barrier to provide not only an ultra-high MR ratio but also an ultra-low RA product in the STT-MTJ, greater than that of the DB system [6, 17, 18].

In this study, ultra-low switching power and small RA product were achieved in the SLB STT-MTJ. Highly efficient spin-dependent transport is one of the essential conditions for developing spintronics technologies. Half-metallic (HM) magnets, for example, Heusler alloys, are one of the most suitable
materials that satisfy these requirements owing to their complete spin polarization at the Fermi energy [19–21]. The insulator layers of the SLB can be made of arbitrary amorphous materials rather than high-quality single-crystalline materials. The combination of HMs and SLBs generates an efficient spin-polarized transport. The RA product of the device can be reduced below 0.2 Ω μm², and the writing power decreases by over 90%. The results exhibit that STT and current features are qualitatively and quantitatively consistent with the theoretical studies [14, 22, 23] and refer to the experiments [14, 24, 25]. Moreover, their excellent advantages imply that HM magnets with exceptional coercivity and magnetocrystalline anisotropy are most suitable for the fixed layer in STT-MTJ devices [26, 27].

2. Model and formulation

An STT-MTJ is a combination of two magnetic layers separated by the SLB, as shown in figure 1. The direction of magnetization in the left magnetic film is fixed (fixed layer), and the direction of the right film is freely rotated at any angle $\theta$ (free layer). The fixed layer can be set as the HM (e.g., full-Heusler alloy Co$_2$MnSi (CMS)) or FM magnets (e.g., CoFeB family). Each electrode has spin-up and spin-down states is freely rotated at any angle $\theta$. Based on boundary conditions presented in references [8, 29], the charge current density can then be derived from the electron transport amplitude of the total electron wave function.

$$\Gamma = \begin{bmatrix} \cos (\theta/2) & -\sin (\theta/2) \\ \sin (\theta/2) & \cos (\theta/2) \end{bmatrix}.$$ Based on boundary conditions presented in references [8, 29], the charge current density can then be derived from the electron transport amplitude of the total electron wave function $\psi_\sigma(y)$, expressed as

$$j^z = \frac{e \hbar}{2m^*} \text{Im} \sum_\sigma \left( \psi_\sigma(y) \left( \frac{d}{dy} \psi_\sigma(y) \right) \right).$$

When the magnetization orientation is considered, the general form of the spin probability flux density is given by $j^z = \frac{\hbar}{2m^*} \left( \left( \frac{d}{dy} \Psi^+ (y) \right) \hat{\sigma} \Psi(y) - \Psi(y) \hat{\sigma} \Psi(y) \left( \frac{d}{dy} \Psi(y) \right) \right)$, where the component $(\epsilon = x, y, z$ or $\epsilon = x', y', z')$ is the local coordinate of the system and $\Psi(y) = \begin{bmatrix} \psi_\uparrow \psi_\uparrow \\ \psi_\downarrow \psi_\downarrow \end{bmatrix}$ is the spinor of the wave functions. According to the formulation, the total spin current density [23] in the zero-temperature approximation
Figure 1. (a) Geometric structure of a three-cell superlattice MTJ, where the yellow layers B indicate the insulator barrier, and the brown layers A indicate the NM metal. The semi-infinite electrode of the left fixed layer can be HM or FM magnets. The right free layer is set as FM. Directions of magnetization $M$ are pointed out by the green arrows, and the spin torque of the free layer depends on the angle $\theta$.

Schematic diagram of the spin-resolved band structure in (b) superlattice- and (c) DB MTJs with spin-up (red arrows) and spin-down (blue arrows) states. A bias voltage is exerted on the device, proportionally.

The total current is obtained based on the entire energy interval from the bottom energy band of the left electrode to the Fermi level. $E_{Lb}$ is the origin of the spin-up energy band for the incident electrode.

According to the spin current density mentioned, the spin torque that acts on the right film is derived from the formula of the spin current with two components, the in-plane (STT) and out-of-plane (normal torque) directions [30]. Hence, the STT and the normal torque (per unit square) of the free layer can be written as $T_{\text{STT}} = -\frac{\hbar}{2} J_s x'$, and $T_{\text{normal}} = -\frac{\hbar}{2} J_s y'$, respectively, including the orientation $\epsilon$. Note that the equations are of the semi-infinite free layer, where a sufficiently thick layer can completely absorb the spin magnetization. When the free layer is considered to be of finite thickness, the STT can be regarded as the difference between the left interface and the right point of the free layer.

$J_s x'$ and $J_s y'$ are the parallel and perpendicular components of the spin current density obtained from equation (6). The contribution to the normal torque given only by the electrons from the energy windows, between the Fermi levels in both the electrodes, is considered.

3. Results and discussion

Initially, the dependence of the current-induced STT and the charge current density, versus thickness of the NM metal in a three-cell SLB MTJ, are shown in figure 2. The parameters of the system are selected as $V_b = 500$ mV, $\theta = \pi/2$, Fermi level $E_F = 2.25$ eV, and $U_B = 1$ eV above the Fermi level. The total length of barriers, $D_B$, is 1.2 nm with $D_B = d_{B1} + d_{B2} + d_{B3}, \ldots + d_{Bn}$, where $n$ indicates the period number in the $n$-cell superlattice system. The magnitude of the right free layer molecular field, related to the FM magnets, is taken as $\Delta_R = S_R/2 = 1.48$ eV. By introducing the characteristics of HMs, the material of the left fixed layer is considered to be HM magnets with $\Delta_L = 2.5$ eV. In practice, from figure 2, it is seen that sharp peaks of the larger STT and charge current density appearing at specific $d_A$ are attributed to the band structure in the SLB. The distribution of band structure in the SLB is divided as allowed bands and forbidden bands. The STT amplitude is enhanced to twice as that in the SLB MTJs, with two FM electrodes. The results can be up to 10 times of magnitude larger than that in the DB-MTJ system, as presented in the previous research [8]. This bandpass phenomenon is considered important in the periodic multilayer systems owing to the manipulation of the electron transport with many realizations of application [31, 32].
Figure 2. Thickness dependence of the (a) STT and (b) charge current density in HM STT-MTJs. The square markers represent the corresponding STT and current density in the DB system. Points A and B indicate the first and second maximum peaks of the three-cell SLB structure, respectively. The total thickness of barriers is denoted as $D_B$.

Figure 3. (a) Switching power with a critical current density of $J_c = 0.1 \, \text{A} \, \mu\text{m}^{-2}$ in the HM MTJ. The maximum power is set by the operating bias and the critical current density in MTJ devices. The square markers represent the corresponding power and RA product in the DB system. Points C and D indicate the minimum power valleys corresponding to first and second maximum peaks in figure 2, respectively. (b) Thickness dependence of RA product in the HM STT-MTJ. The properties of the DB system and the two-cell SLB are the same order of magnitude. Moreover, when the thickness, $d_A$, shifts away from the maximum peak, the STT decreases drastically. As depicted in figure 2(a), a maximum STT of up to 5000 eV $\mu$m$^{-2}$ is almost 500 times larger than that of the MgO-based MTJs, considering HM electrode in this three-cell SLB system [22, 23]. Simultaneously, the current features are noticeably enhanced because of the passband (point A and point B), which is advantageous for data writing on the STT-MRAM. Remarkably, the second maximum peak of the STT reaches about 2300 eV $\mu$m$^{-2}$ with a thicker $d_A$, which is more realizable in experimental fabrication.

When the critical current of magnetization switching is set to 0.1 A $\mu$m$^{-2}$, the diagrams of the switching power are shown in figure 3(a). Points C and D indicate the first and second minimum power valleys corresponding to the first and second maximum peaks in figure 2, respectively. The power at the second valley, point D, is below 0.01 W $\mu$m$^{-2}$. The passbands of the SLB can allow a large number of electrons to pass through the system, which causes very high STT and current density peaks. The magnetization is more likely to be switched in this low-power condition. Compared to the condition of point D, the thickness of point C is significantly thin to the extent that it is difficult to adopt in practical applications. The RA product, as a function of $d_A$, is also plotted in figure 3(b), which shows that the RA product sharply decreases to a minimum of approximately 0.2 $\Omega$ $\mu$m$^2$ with low power, as indicated by point D. The value is less than 10% of the RA in traditional single-barrier (SB) MTJs. Therefore, the SLB structure can effectively enhance the performance of the MTJs.

Next, the in-plane and normal components of spin-torque versus the angle with $d_B = 0.4$ nm are shown in figure 4(a) to understand the variations in more detail. The lower left inset shows an enlarged figure of the corresponding results for the HM and FM electrodes in the SB system. The component of the in-plane torque is significantly larger than the normal torque. This is different from the features of the traditional MTJ, where the components of both the in-plane torque and normal torque are of comparable order in magnitude, as seen in figure 4(a). From figure 2, it is found that the STT and the charge current density increase as the $d_A$ approaches the peak. The STT exhibits sinusoidal oscillation, approaching the maximum amplitude at $\theta = \pi/2$ (and $\theta = 3\pi/2$), and is maintained at zero in the collinear configuration. The magnetization direction of the free electrode is perpendicular. The thicknesses of the NM metal, $d_A$, from
Figure 4. (a) Torque of the in-plane component versus deflection angle of free layer with fixed $d_b = 0.4$ nm. The inset in the lower-left corner is an enlarged graph of the STT with $d_A = 0$ nm (SB system). The right insets show the normal torque in the MTJ. (b) Charge current density versus angle in different thicknesses of the NM metal. The inset exhibits the enlarged graph of the current density in the SB system for the HM and FM electrodes.

Figure 5. Bias dependence of the (a) STT and (b) charge current density for four different conditions of the NM-metal layer. The red curve is selected as the second peak in figure 2. (c) Enlarged graph shows the bias dependence of the charge current density in the SLB MTJ with small bias voltages. The magenta dashed line shows the critical current density of $10^7$ A cm$^{-2}$ in typical MTJ devices. All the parameters are the same as those in figure 4, except the angle, $\theta = \pi/2$.

0.4 to 0.45 nm are depicted in figure 4 owing to the relevance of the peak and valley locations. The STT, with the maximum amplitude up to 2400 eV$\mu$m$^{-2}$, is attenuated as the thickness of the metal layer increases slightly, as shown in figure 2. When $d_A$ shifts from 0.38 nm to 0.45 nm, where the allowed band is a contraction, the charge current density reaches the maximum in the parallel configuration ($\theta = 0$) and monotonically decreases to the valley, as the direction moment rotates toward the antiparallel configuration ($\theta = \pi$). This phenomenon qualifies as the standard of tunneling junctions. However, the charge current density is almost insusceptible in a special case with the angle variation when $d_A = 0.38$ nm. This property can be attributed to the dominance of the spin-up electrons in the SLB because of HM characters, as seen in the discussion in figure 6. The results calculated for the junctions significantly influence the band modulation of the barrier height and the SLB distribution. Accordingly, the primary contribution of the current is controlled by the spin-up transport (with a strong bandpass), instead of both the spin-polarized states of electrons. Hence, when $d_A = 0.38$ nm, the charge current is larger than that under other conditions. Furthermore, it is seen that the normal torques are very small, lower than four times that of the in-plane torque. Notably, when the structure is set at $d_A = 0$ nm (traditional MTJ), the HM electrode enhances the STT by a factor of 12, compared to FM-based MTJs, as seen in the inset. Simultaneously, the current density is reduced to nearly half of that in the FM one. The results are considered to be the dominant HM properties of the strong spin-polarized electrons and the interaction between the barrier and the spin electrons [23].

Finally, the bias dependence of the STT and the charge current density are investigated with a deflection angle of $\theta = \pi/2$. The enlarged graphs of the STT and the charge current density in the uncomplicated SB-MTJ, with HM and FM fixed layers, are depicted in the insets of figures 5(a) and (b). The critical current density in the traditional SB system, corresponding to the evidential references [24, 25], is illustrated by the magenta dashed line in figure 5(c). Compared with the SB-MTJs, the system can be easily operated at a small bias voltage of about 24 mV with a very low switching power. More significantly, with regard to the traditional SB-MTJs reported in the prior study, the results reveal that the switching power decreased to less than 10%, compared with reference [11]. It is obvious that ultra-low switching power is achieved in this
HM system. Considering the SB structure, the torque of the free layer is strongly influenced by the tunneling efficiency of electron transport, which depends on the effective spin polarization of the magnetic electrode. While the STT increases more rapidly than that of the traditional SB-MTJ for large bias voltages using the HM free layer, the current relatively decreases. For the FM/B/FM structure, the sign of the STT suffers from the influence of the barrier height and (negative) bias voltage. The variations in the corresponding barrier height create a sign change for effective spin polarization. However, a distinctively different trend is exhibited in the SLB system, as shown in figures 5(a) and (b). The spin polarization of electrons in the SLB structure is successfully steadied with regard to the asymmetry of the spin states and barrier influence. Hence, as shown by the red curve in figure 5(a), the magnitude of the maximum STT is 8000 times larger than that in the SB system with the HM electrode and larger than five orders of magnitude in the FM-based MTJ without any sign change. To sum up, combining the suitable SLB spacer and the characteristics of the HM magnets not only significantly contributes to the stability of the spintronics devices but also greatly advances the efficiency of the system.

The band structure of the SLB strongly influences the transport properties of the MTJ. To determine the reason for the huge STT and low RA product, the transmission spectra of the spin-up and spin-down electrons are shown in figure 6. The green channels, in figure 6, represent the allowed bands in the three-cell SLB. The transmission probabilities are calculated under the conditions of the second STT peak and valley for \( d_A = 0.38 \) nm and 0.5 nm, respectively. Compared with the traditional FM electrode MTJ, the proposed HM structure is more influenced by the spin-up polarization than the spin-down electrons. These transmission peaks are observed in the energy channel of the corresponding allowed bands that are formed by the SLB structure. In figure 6(a), the second allowed band significantly contributes to the spin-polarized current, where the transmission probability approaches 1. The first transmission peaks offer a limited contribution, as shown in figure 6(a). Figure 6(b) shows the condition of the lower STT and the current valley for \( d_A = 0.5 \) nm. It is clearly seen that only the transport channel (allowed band) appears at the center of the entire energy region. This phenomenon leads to a restriction on transport based on the narrow allowed band. Hence, it is found that the features of the STT and current density are ordinary in this condition. Moreover, the transmission probability of the spin-down polarization is approximately 12 orders lower than that of figure 6(a) in the forbidden band, which is very unfavorable for spin transport.

4. Conclusions

In conclusion, an ultra-low switching power below 10% of the MgO-barrier MTJ can be achieved using the properties of the HM magnet and the SLB. The system can be operated at minimal power with sufficient switching current and STT. For a prescribed set of stable operating conditions, the STT effect exceeding 500 times that of the traditional MgO-based MTJ is attainable with high spin polarization and a strong bandpass phenomenon. Spin-polarized currents and switching efficiency of the device can be significantly enhanced by the high spin polarization of the HM electrode. The RA product of the device is noticeably reduced to \( 0.2 \, \Omega \, \mu \text{m}^2 \), which is less than 10% of that in the MgO-based MTJs. Furthermore, since stable amorphous rather than high-quality crystalline is used in the SLB structure, the degradation caused by the repeated writing on the STT-MTJs can be avoided. Thus, the MTJ system can provide greater reliability and endurance. The proposed device can not only reduce the influence of Joule heating but also protect the endurance of the MTJs, with respect to the reduction of the switching power.
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