Simulation of stress-modulated magnetization precession frequency in Heusler-based spin torque oscillator

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Abstract

We investigated stress-modulated magnetization precession frequency in Heusler-based spin transfer torque oscillator by combining micromagnetic simulations with phase field microelasticity theory, by encapsulating the magnetic tunnel junction into multilayers structures. We proposed a novel method of using an external stress to control the magnetization precession in spin torque oscillator instead of an external magnetic field. The stress-modulated magnetization precession frequency can be linearly modulated by externally applied uniaxial in-plane stress, with a tunable range 4.4~7.0 GHz under the stress of 10MPa. By comparison, the out-of-plane stress imposes negligible influence on the precession frequency due to the large out-of-plane demagnetization field. The results offer new inspiration to the design of spin torque oscillator devices that simultaneously process high frequency, narrow output band, and tunable over a wide range of frequencies via external stress.

Keywords: spin torque oscillator, magnetization precession frequency, micromagnetic simulation, Heusler alloys

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1. Introduction

Since the prediction of spin transfer torque (STT) ^{1,2} that a spin-polarized electron can transfer the angular momentum to the ferromagnetic magnetization, many different spin torque oscillators (STO) configurations have been investigated to obtain the magnetization oscillation ³⁻⁶. Coupled with the giant magnetoresistance effect (GMR) ⁷⁻⁹, this stable magnetization precession produces a voltage response that makes these devices high-frequency oscillators. ¹⁰ STO provides many attractive advantages, e.g., high frequency microwave, narrow output band with high Q values, tunable over a wide range of frequencies via applied field or current, and voltage outputs in the mV regime. ¹¹, ¹² However, the lower output power of metal STO is the biggest problem for designing applicable devices. Recently, the high polarization materials like Heusler alloys with lower saturation magnetization M_s , ¹³ smaller Gilbert damping constant α , ¹⁴ higher spin polarization factor η ¹⁵ and higher GMR ratio ^{16,17} are used, it can increase GMR signal and hence the power output from the oscillator. For example, a high output power of 1.1 nW ^{18,19} were achieved in Heusler Co_2MnSi (CMS) alloy.²⁰ Except the half-metallic properties with high polarized constant, Heusler alloys also have giant magnetostrictive effects. An applied magnetic field can re-orientate the ferroelastic domains, and obtain giant strains an order of magnitude higher than those of giant magnetostrictive materials. In Heusler alloy Ni_2MnGa tetragonal five-layered and orthorhombic seven-layered martensitic phases, martensitic strains of about 60000 and 95000 ppm have been produced by a magnetic field, respectively. Therefore, we import the giant magnetostrictive effects into current-induced magnetization oscillation in Heusler-based magnetic tunnel junction structures. In addition, the substrate misfit strain was

demonstrated to effectively decrease the critical current density of magnetization switching²¹⁻²³. Therefore, we propose the external stress to modulate the magnetization precession frequency in Heusler-based STO devices. Furthermore, the narrowing optimum current region for the magnetization oscillation due to the high spin polarization constant of Heusler alloy limits the frequency tunability.^{24, 25} The balance between STT and the damping torque is the key to stabilize the precessional oscillation, the magnitude of the effective field is not sufficiently large to compete with the large STT originating from the high spin polarization constant in Heusler-based spin valve nanopillars.²⁶⁻²⁸ Here, we introduce the external stress to increase or decrease the effective field, thus widen frequency tunability.^{23, 29, 30}

In this paper, we investigated stress-control magnetization precession frequency in Heusler-based STO by combining traditional micromagnetic simulations with phase field microelasticity theory. We argue that one can utilize the external stress to tunable widely the magnetization precession frequency instead of the external magnetic field or current density. In addition, the frequency tunability of STO in the absence of an external magnetic field enables the integration of STO and conventional complimentary metal-oxide semiconductor devices.

2. Methods

We use a generalized Landau-Lifshitz-Gilbert-Slonczewski (LLGS) equation to describe magnetization $\mathbf{M}$ dynamics,^{1, 2}

$$\begin{aligned} \frac{d\mathbf{M}}{dt} = & -\gamma' \mathbf{M} \times \mathbf{H}_{eff} - \frac{\alpha \gamma'}{M_s} \mathbf{M} \times (\mathbf{M} \times \mathbf{H}_{eff}) - \frac{2\mu_B J}{(1 + \alpha^2) e d M_s^3} g(\mathbf{M}, \mathbf{P}) \mathbf{M} \times (\mathbf{M} \times \mathbf{P}) \\ & + \frac{2\mu_B \alpha J}{(1 + \alpha^2) e d M_s^2} g(\mathbf{M}, \mathbf{P}) (\mathbf{M} \times \mathbf{P}) \end{aligned} \quad (1)$$

where $\gamma' = \gamma/(1+\alpha^2)$, γ is the electron gyromagnetic ratio, α is the dimensionless damping parameter, and $\mathbf{H}_{eff}$ is the effective field. The last two terms on the right side of Eq. (1) describe STT that tend to drag the magnetization away from its initial state to its final state. μ_B , J , d , e , M_s , are the Bohr magneton, current density, thickness of the free layer, electron charge, and saturation magnetization, respectively. The scalar function is given by,^{1, 2}

$$g(\mathbf{M}, \mathbf{P}) = [-4 + (1 + \eta)^3 (3 + \mathbf{M} \cdot \mathbf{P} / M_s^2) / 4\eta^{3/2}]^{-1} \quad (2)$$

where η is the spin polarization constant, $\mathbf{M}$ and $\mathbf{P}$ are the magnetizations of free and fixed layers, the angle between $\mathbf{M}$ and $\mathbf{P}$ is θ . $\mathbf{M} \cdot \mathbf{P} / M_s^2 = \cos \theta$.

The effective field is calculated by,

$$\mathbf{H}_{eff} = -\frac{1}{\mu_0} \frac{\delta E}{\delta \mathbf{M}} \quad (3)$$

where E is the total energy, expressed by $E = E_k + E_d + E_{ext} + E_{elas} + E_{ex} + E_{stt}$, where E_k , E_d , E_{ext} , E_{elas} , E_{ex} , E_{stt} are anisotropy energy, demagnetization energy, Zeeman energy, elastic energy, exchange energy, and STT energy, respectively. The details for obtaining E_k , E_{ext} , E_{ex} and E_{stt} can be found in Ref. 31.³¹ In Park et al.'s work³², the effective field is represented as, $\mathbf{H}_{eff} = \mathbf{H}_{shape} + \mathbf{H}_{stress}$, the elastic field is not considered and the effective field is modified by adding the stress-induced term. However, the effective field in our work is given as, $\mathbf{H}_{eff} = \mathbf{H}_k + \mathbf{H}_d + \mathbf{H}_{ext} + \mathbf{H}_{elas} + \mathbf{H}_{ex} + \mathbf{H}_{stt}$, including the anisotropy field, the demagnetization field, the external field, the elastic field, the exchange field and the STT field.

A finite size magnet magnetostatic boundary condition is applied to calculate the demagnetization energy E_d , to consider the influence of geometric size on the magnetic domain structures. The magnetostatic energy density E_d can be written as,³³

$$E_d = -\frac{1}{2}\mu_0 (\mathbf{H}_d^{\text{tot}} \cdot \mathbf{M}) \quad (4)$$

$$\mathbf{H}_d^{\text{tot}} = \mathbf{H}_d^{\text{hetero}}(\mathbf{M}) + \mathbf{H}_d^{\text{shape}}(\overline{\mathbf{M}}) .$$

Here the total stray field $\mathbf{H}_d^{\text{tot}}$ consists of a heterogeneous contribution $\mathbf{H}_d^{\text{hetero}}(\mathbf{M})$ and an demagnetization part $\mathbf{H}_d^{\text{shape}}(\overline{\mathbf{M}})$, which are obtained by solving the magnetostatic equilibrium equation, i.e., $\nabla \cdot (\mu_0 \mathbf{H}_d^{\text{hetero}} + \mu_0 M_s \mathbf{M}) = 0$ and $\mathbf{H}_d^{\text{shape}}(\overline{\mathbf{M}}) = \mathbf{N}\overline{\mathbf{M}}$, respectively. $\mathbf{N}$ is the sample-shape dependent demagnetizing factor matrix.

In particular, the elastic energy E_{elas} is calculated based on a previously developed phase-field model³⁴ for a three-phase system that is comprised of an isolated magnetic film (the free layer herein), a stiff substrate, and the air. The elastic energy can be expressed by,³⁵

$$E_{\text{elas}} = \frac{1}{2} \int c_{ijkl} e_{ij} e_{kl} dV = \frac{1}{2} \int c_{ijkl} (\varepsilon_{ij} - \varepsilon_{ij}^0)(\varepsilon_{kl} - \varepsilon_{kl}^0) dV \quad (5)$$

where the summation convention is employed and $i, j, k, l = 1, 2, 3$. c_{ijkl} is the elastic stiffness tensor, e_{ij} is the elastic strain, and

$$\varepsilon_{ij}^0 = \frac{3}{2} \lambda_{100} (m_i m_j - \frac{1}{3}) \quad (i = j) \quad \text{or} \quad \frac{3}{2} \lambda_{111} m_i m_j \quad (6)$$

where λ_{100} and λ_{111} are the magnetostrictive constants, and $\mathbf{m} = \mathbf{M}/M_s$. In this system, a homogeneous applied stress is loaded, the total potential energy is given by the sum of elastic energy of the system and the potential of the mechanical loading,

$$E_p = E_{\text{elas}} - V \sigma_{ij} \overline{\varepsilon_{ij}} \quad (7)$$

After minimizing the total potential energy with respect to the homogeneous strain, we can obtain,

$$\overline{\varepsilon}_{kl} = \frac{1}{V} \int \varepsilon_{kl}^0 dV + s_{ijkl} \sigma_{ij} \quad (8)$$

where s_{ijkl} is the elastic compliance tensor. Using Eq. (7), we obtain the homogeneous strain:

$$\begin{aligned} \overline{\varepsilon}_{11} &= s_{11} \sigma_{11} + s_{12} (\sigma_{22} + \sigma_{33}) + \frac{3}{2} \lambda_{100} (\overline{m_1^2} - \frac{1}{3}) \\ \overline{\varepsilon}_{12} &= \frac{1}{2} s_{44} \sigma_{12} + \frac{3}{2} \lambda_{111} \overline{m_1 m_2} \\ \overline{\varepsilon}_{22} &= s_{11} \sigma_{22} + s_{12} (\sigma_{11} + \sigma_{33}) + \frac{3}{2} \lambda_{100} (\overline{m_2^2} - \frac{1}{3}) \\ \overline{\varepsilon}_{13} &= \frac{1}{2} s_{44} \sigma_{13} + \frac{3}{2} \lambda_{111} \overline{m_1 m_3} \\ \overline{\varepsilon}_{33} &= s_{11} \sigma_{33} + s_{12} (\sigma_{11} + \sigma_{22}) + \frac{3}{2} \lambda_{100} (\overline{m_3^2} - \frac{1}{3}) \\ \overline{\varepsilon}_{23} &= \frac{1}{2} s_{44} \sigma_{23} + \frac{3}{2} \lambda_{111} \overline{m_2 m_3} \end{aligned} \quad (9)$$

where s_{11} , s_{12} , and s_{44} are the three independent compliance constants for a cubic material in the Voigt's notion.

The dynamics of magnetization is investigated by numerically solving the time-dependent LLGS equation using the Gauss-Seidel projection method with a constant time step $\Delta t = 0.0268858$ ps.³⁶⁻³⁸ We adopted the following magnetic parameters, magnetocrystalline anisotropy constant $K_1 = 3.0 \times 10^3$ J/m³, and $K_2 = 0$,³⁹ exchange constant $A = 2.0 \times 10^{-11}$ J/m,⁴⁰ saturation magnetization $M_s = 8.0 \times 10^5$ A/m.⁴¹ Other parameters are Gilbert damping parameter $\alpha = 0.008$,¹⁴ spin polarization factor $\eta = 0.56$,^{42, 43} electron gyromagnetic ratio $\gamma = 2.3245 \times 10^5$ m/(A·s), elastic constants $c_{11} = 3.16 \times 10^{11}$ N/m², $c_{12} = 1.74 \times 10^{11}$ N/m², $c_{44} = 1.43 \times 10^{11}$ N/m²,⁴⁴ magnetostrictive constants $\lambda_{100} = 12.22 \times 10^{-6}$, and $\lambda_{111} = 0$.^{45, 46}

3. Results and Discussion

Figure 1 (a) shows a schematic structure of magnetic tunnel junction with CMS (16 nm)/MgO (2 nm)/CMS (2 nm) and the square cross section area of $64 \times 64 \text{ nm}^2$. The top and bottom CMS layers are the fixed and free layers, and the middle MgO layer is an insulator. The bottom substrate is ferroelectric materials to provide the external stress which is controlled by the magnitude of voltage. In our simulation, a positive current is defined as a current flowing from the free layer to the fixed layer, and the electrons will be polarized by the magnetization of the fixed layer. The polarized electrons tunnel the insulator layer MgO, and the STT will act on the free layer magnetization. The initial magnetization vector $\mathbf{M}$ of the free layer is along the negative x axis, while the initial magnetization $\mathbf{P}$ along the positive x axis. Figure 1 (b) shows the free layer under the loading of applied stress at different directions along x , y , and z axes. At a small current density, the damping torque will push $\mathbf{M}$ back toward the low energy configuration along the negative x axis. With the increase current density, a stable magnetization precession will be produced as STT input equals to the magnetic damping torque.

Figure 2 (a) shows the temporal evolution of magnetization components $\langle m_x \rangle$ at the current density of $4.0 \times 10^6 \text{ A/cm}^2$ and the external stress of zero stress, 10 MPa, and -10 MPa, respectively. For clarify, the components $\langle m_x \rangle$ shift up with 0.5 and 1.0 under the external stress of 10 MPa and -10 MPa, respectively. As seen, the magnetization precession under the negative stress of -10 MPa has a short initial oscillation which results from the stimulation of external stress. In contrast, the positive stress of 10 MPa prolongs the initial oscillation. The phenomena are resulted from the external stress to change the magnitude of initial effective field along $-x$ axis. Therefore, we demonstrate

that the external stress can speed up the magnetization oscillation by decreasing the initial oscillation to increase the efficiency of STO. For detail illustration, Figure 2 (b) shows the temporal evolution of three magnetization components $\langle m_x \rangle$, $\langle m_y \rangle$, and $\langle m_z \rangle$ in the zooms of time span from 25.0 to 25.5 ns. The oscillation frequency of $\langle m_x \rangle$ is approximately twice as large as that for $\langle m_y \rangle$ and $\langle m_z \rangle$ oscillation, because the $\langle m_x \rangle$ component moves back and forth twice during one complete precession cycle. As shown in Figure 2 (c), the four snapshots of magnetization distributions in the x - y plane correspond to the four points in the temporal evolution of magnetization. The arrows indicate the magnetization. The magnetization almost entirely lies in the x - y plane during the entire oscillation showing uniform magnetization precession. In addition, we also show the magnetization precession trajectory in Figure 2 (d).

As shown in Figures 3 (a)-(c), we show the power spectrum density (PSD) at different directions and magnitudes of external stress and same current density of $4.0 \times 10^6 \text{ A/cm}^2$. For clarify, the PSD of y axis shifts up with 0.5 each curve with the increase of external stress. For the x axis stress σ_{11} , the frequency is increasing with the increase of external stress. In contrast, the frequency is decreasing with the y -axis external stress σ_{22} . The frequency is not influenced by the z -axis external stress σ_{33} since the large demagnetization field along z axis due to the magnetic thin film. We summarize our results that the external stress plays different roles in the magnetization precession by using Figure 3 (d). Therefore, we demonstrated that both x and y axes external stresses can overcome the limit range of magnetization precession and broaden the oscillation range in the Heusler-based STO. In addition, we proposed that one can use the external stress to adjust the frequency of STO.

For detail illustration, we analyzed the influence of x axis external stress to the effective field as an example. As shown in Figures 4 (a) and (b), we show the evolutions of total effective fields and elastic effective field along x axis at the current density of $4.0 \times 10^6 \text{ A/cm}^2$ and zero stress, 10 MPa , and -10 MPa . As seen, the negative external stress increases the effective field, but the positive decreases. Since the frequency is proportional to the effective field along $-x$ axis. If the x -axis stress is applied to the film, the effective field will increase with the magnitude of the stress. However, the negative x -axis stress is applied, the effective field will decrease. Therefore, we obtain that the frequency has a linear relationship with the external stress which are similar to the frequency dependence on the external magnetic field. As seen, the elastic effective field plays a significant role during the magnetization precession. We also show the projection of magnetization trajectories on y - z and x - z planes in Figures 4 (c) and (d). With the effect of external stress, the magnetization precession can be enlarged or pressured at different directions of external stress.

In order to understand the influences of external stress to the magnetization precession, we calculated the phase diagrams of magnetization dynamics under the external stress. Figure 5 shows the phase diagram of the magnetization as a function of current and external stress along x axis. The blue and red colors also represent the magnetization along $-x$ and $+x$ axe, respectively. The stress along the positive x axis favors the parallel configuration while a stress along the negative x axis impedes the parallel configuration. If we apply the stress along the positive x axis, the blue area increases gradually while a stress is applied along the negative x axis is applied, the blue area decreases gradually. Therefore, the optimum current range for spin transfer

precession can be increased or decreased depending on the direction of an external stress. In short, both the external stress and magnetic field (see figure 5 in Ref. 28) can adjust the magnitude of the effective fields, and the magnetization precession frequency can be shifted by applying either an external magnetic field or stress. However, stress-modulated oscillation frequency can simplify STO devices since the magnetic field-modulated oscillation frequency needs additional device to produce the magnetic field.

4. Conclusions

In conclusion, we investigated stress-control current-induced magnetization precession in CMS-based magnetic tunnel junctions by combining phase field simulations with micromagnetic simulations. An effective method of stress control magnetization frequency is proposed to adjust the magnitude of effective field and widen the magnetization frequency range instead of an external magnetic field. The precession time of magnetization is reduced by introducing the external stress, and the precession frequencies are linear with the external stress in the plane, and independent with the external stress out-of-plane. The results offer new inspiration to the design of STO devices that simultaneously possess high frequency, narrow output band, and tunable over a wide range of frequencies via external stress.

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Figure Captions

Figure 1 (a) Structure of magnetic tunnel junction structures (b) Free layer under external stress.

Figure 2 (a) The temporal evolution of magnetization components at the external stress and current density of $4.0 \times 10^6 \text{ A/cm}^2$. (b) The zoom of time span from 25.0 ns to 25.5 ns. (c) Snapshots of magnetization distribution. (d) Magnetization precession trajectory.

Figure 3 Power spectrum density under the stress along (a) x , (b) y , and (c) z axes. (d) Magnetization precession frequency shift under stress along x , y and z axes.

Figure 4 The temporal evolutions of (a) total effective field and (b) elastic effective field on the x axis. The projections of magnetization precession trajectories on (c) y - z plane and (d) x - z plane.

Figure 5 Phase diagram showing the magnetization as a function of applied current density and external stress along the x axis.