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Implementation of one-dimensional domain wall dynamics simulator

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We implemented a one-dimensional domain wall (DW) dynamics simulator based on the well-developed collective coordinate approach to demonstrate DW motion under a given magnetic field and/or current flow. The simulator adopted all known influences, including three-dimensional external magnetic fields, spin transfer torque with non-adiabatic contribution, spin Hall effect, Rashba effect, and Dzyaloshinskii-Moriya interaction. The simulator can calculate the position, velocity, internal magnetization angle, and tilting angle of the domain wall to the current direction or wire axis under given simulation conditions and material parameters. It will not only provide physical insights of domain wall dynamics to experimentalists, but also can be used to more easily simulate various physical circumstances before running time-consuming micromagnetic simulations or real experiments.
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I. INTRODUCTIONS

Since the proposal of domain wall (DW) motion based memory devices[1] and the discovery of DW motion induced by spin transfer torque (STT),[2] various techniques for manipulation of DW position have been studied.[3–11] Once the concept of race track memory has been proposed, DW motion by STT has been heavily investigated. There are many debates about the role of non-adiabatic torque.[12,13] Several field-driven DW motion ideas such as perpendicular magnetic field pulse for in-plane DW,[7] ac magnetic field in ratchet type nanowire,[8] asymmetric potential energy,[9] and non-uniform magnetic field[10,11] have also been suggested. A decade ago, several other sources of spin torque, including Rashba effect[3] and spin Hall effect (SHE),[4] were found in heavy metal (HM)/ferromagnetic layer (FM) hetero-structures. Since physical origins of such exotic torques are strong spin-orbit coupling, they are called spin-orbit torque (SOT). SOT has paved a novel way to manipulate DW motion in nanowires and switch the magnetic free layer which is useful for fast three terminal memory devices based on SOT.[14] DW motion is more complicated than SHE and Rashba effects since SOT acts like longitudinal and/or transverse effective fields on the DW.[15,16] More recently, it has been emphasized that Dzyaloshinskii-Moriya interaction (DMI)[17] plays an important role in DW dynamics.[4,16,18,19] Since DMI gives an effective field to enforce Neel-type DW and suppress Walker breakdown, faster DW motion can be achieved.

In order to understand the details of DW motion by external field, STT, and SOT with DMI, proper micromagnetic simulation studies are essential with all effects.[20,21] However, widely used micromagnetic simulator requires careful manipulation of script file in order to handle SOT effect correctly. Furthermore, micromagnetic simulation requires certain amount of simulation resources including computation time. Especially, when the number of adjustable physical parameters is large,

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it is very time consuming, making it difficult to obtain physical insights. Micromagnetic simulation also requires heavy post-processing to extract desired physical results such as DW position, velocity, structures, and so on.

It is known that collective coordinate approach is a simpler method that can solve one-dimensional DW motion[10,22,23] for given material and structural parameters with external magnetic fields, STT, SOT, and DMI terms.[4,18,19] Because the collective coordinate approach oversimplifies DW motion problems, it may ignore some important physical features including the creation of Bloch line[24] and distortion of DW shape. Despite its weakness, it is widely used due to its many benefits such as simplicity and transparent physics.

In this study, we implemented a one-dimensional DW motion simulator using the collective coordinate approach based on Martinez's report.[19] Although solving the collective coordinate method for the DW motion might be trivial, it is not easy for many experimentalist and students because it requires lots of knowledge and efforts in programming. The purpose of the presented study is to present the implementation and distribution[25] of standalone one-dimensional DW motion simulator for someone who needs it. It is very light and handy. One can easily obtain DW position, velocity, and internal magnetization angles such as two tilting angles for given simulation conditions. We believe that this simulator will be very useful for DW motion studies.

II. COLLECTIVE COORDINATE APPROACH FOR ONE-DIMENSIONAL DW MOTION

In this work, we implemented a standalone one-dimensional DW motion simulator based on Martinez's report.[19] We briefly reviewed the one-dimensional model as follows. In this implementation, we took three dimensional external fields (STT, SOT, and DMI) into account to simulate DW behaviors without implementing effects of pinning or thermal agitation. We also considered three degrees of freedom of the DW:[19,26] DW position $X = X(t)$ along the wire axis, DW angle $\Phi = \Phi(t)$, and DW tilting angle $\chi = \chi(t)$ as a function of simulation time. Here, DW angle Φ is the internal magnetization angle of the DW ($\Phi = 0$ or π for Neel type and $\Phi = \pi/2$ or $3\pi/2$ for Bloch type DWs). It is well-known that Φ is a constant before Walker breakdown occurs. However, it varies continuously after Walker breakdown. The third degree of freedom is DW tilting angle χ which is defined by the angle between the normal vector of DW plane and the wire axis. Definitions of these two angles and the coordinate system are shown in Fig. 1. We used almost the same notation of Ref. 19 in order to avoid unnecessary confusion in the present simulator. Definitions of other input material and physical parameters for the simulation are summarized in Table I. All other parameters are automatically calculated inside the simulator.

Equations of motion for one-dimensional DW dynamics are shown below:[19]

$$\left(1+\alpha^2\right)\dot{X} = \frac{\Delta}{\cos\chi}\left(\Omega_A + \alpha\Omega_B\right). \tag{1}$$

$$\left(1+\alpha^2\right)\dot{\Phi} = -\alpha\Omega_A + \Omega_B. \tag{2}$$

$$\dot{\chi} = \frac{\left(\frac{6\gamma_0}{\alpha\mu_0 M_s \Delta\pi^2}\right)}{\tan^2\chi + \left(\frac{L_y}{\pi\Delta\cos\chi}\right)^2}\left[-\sigma\sin\chi + \pi QD\sin\left(\Phi-\chi\right) - \mu_0 H_K M_s \Delta\sin 2(\Phi-\chi)\right]. \tag{3}$$

where Ω_A and Ω_B are given by

$$\begin{aligned}\Omega_A = &-\frac{1}{2}\gamma_0 H_K \sin 2(\Phi-\chi) - \frac{\pi}{2}\gamma_0\left(H_y + H_R\right)\cos\Phi + \frac{\pi}{2}\gamma_0 H_x \sin\Phi \\ &+ \frac{\pi}{2}\gamma_0 H_D \sin\left(\Phi-\chi\right) + \frac{b_J}{\Delta}\cos\chi.\end{aligned} \tag{4}$$

$$\Omega_B = \gamma_0 Q H_z + \frac{\pi}{2}\gamma_0\left(QH_{SH} - \xi H_R\right)\cos\Phi + \xi\frac{b_J}{\Delta}\cos\chi. \tag{5}$$

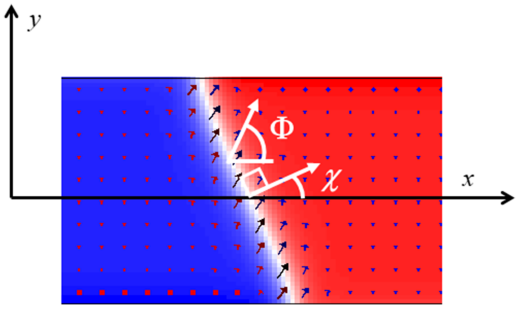

FIG. 1. Definitions of DW angle Φ and DW tilting angle χ with corresponding coordinate system. Results of OOMMF simulations are also shown.

DW energy density with DMI and external magnetic field is given below:

$$\sigma\cos\chi = 4\sqrt{A_{ex}K_u} - Q\pi D\cos(\Phi-\chi) + \mu_0 H_K M_s \Delta\cos^2 2(\Phi-\chi) - \pi\mu_0 M_s\Delta\left[\left(H_y + H_R\right)\sin\Phi + H_x\cos\Phi\right]. \quad (6)$$

Here, $H_K = N_x M_s$ is an effective shape anisotropy field with demagnetization factor N_x. Effective Rashba field, $H_R = \frac{\alpha_R P j_a}{\mu_0\mu_B M_s}$, effective spin Hall field, $H_{SH} = \frac{\mu_B\theta_{SH} j_a}{\gamma_0 e M_s L_z}$, and effective DMI field, $H_D = \frac{D}{\mu_0 M_s\Delta}$ are internally defined in the simulator. More details are explained in Ref. 19. The simulator solves the above coupled three 1st order differential Eqs. (1), (2), and (3) using ODE45 solver in MATLAB for a given time interval is using explicit Runge-Kutta method. DW velocity is obtained from calculated DW positions.

III. USAGE OF THE SIMULATOR

Figure 2 shows an input dialog box of the simulator. In the dialog box, one can find ferromagnetic material parameters, heavy metal material parameters, DW properties, and simulation (running) parameters. Physical meanings of each parameter are explained in Table I. These parameters can be saved as text file (*.txt) which can be edited with any text editor. They can be opened in the simulator for next simulations. The simulator can be run in two current density modes: fixed (one) current density and multiple current densities. When inputs for the current density step and stop are zero, the simulator runs only for a given current density. However, when these have non-zero values, the simulator calculates multiple DW motions for each current density. The output dialog

TABLE I. Definition of input material and physical parameters in the simulator.

Parameters	Physical meaning	Unit
α	damping constant	dimensionless
M_s	saturation magnetization	A/m
D	DMI energy density	J/m^2
A_{ex}	exchange stiffness constant	J/m
K_u	uniaxial anisotropy energy	J/m^3
P	spin polarization	dimensionless
ξ	non-adiabatic parameter	dimensionless
θ_{SH}	spin Hall angle	radian
α_R	Rashba parameter	eV m
η	non-adiabatic Rashba term	dimensionless
Q	+1 for up-down, -1 for down-up DW	dimensionless
L_y, L_z	width & thickness of nanowire	m
B_x, B_y, B_z	External field for x, y, and z direction	T
j_a	current density	A/m^2

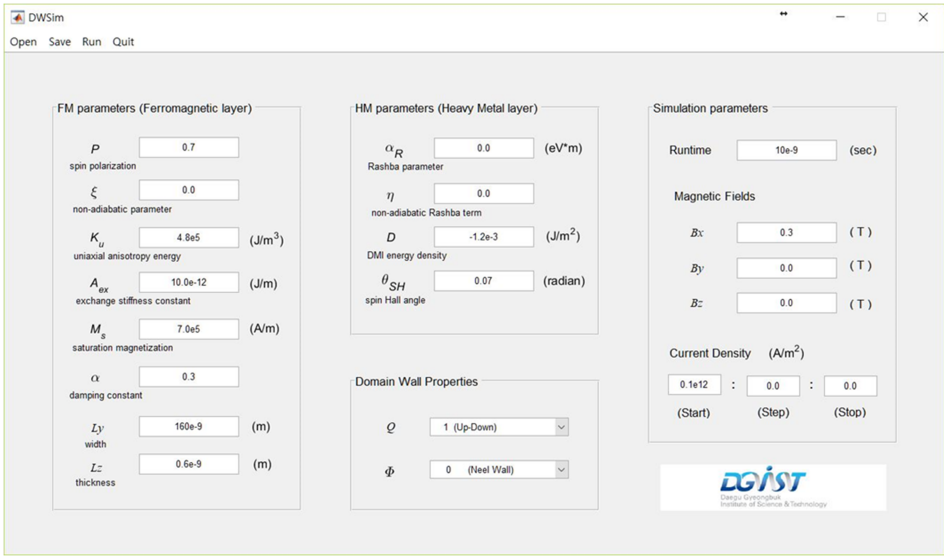

FIG. 2. The input dialog box of the simulator. Ferromagnetic properties, heavy metal properties, DW properties, and simulation parameters can be edited and saved.

box consists of four plots as shown in Fig. 3. The top left panel is DW position. The top right panel is DW velocity. The bottom left panel is Φ (internal magnetization angle) and the bottom right panel is χ (DW tilting angle) as a function of time. Calculated results can be saved as text file with five columns: simulation time, DW position, DW velocity, Φ (internal magnetization angle), and χ (DW tilting angle), respectively. For multiple calculations for various current densities, output file names are saved with sequential numbers. Results of multiple current densities are plotted together

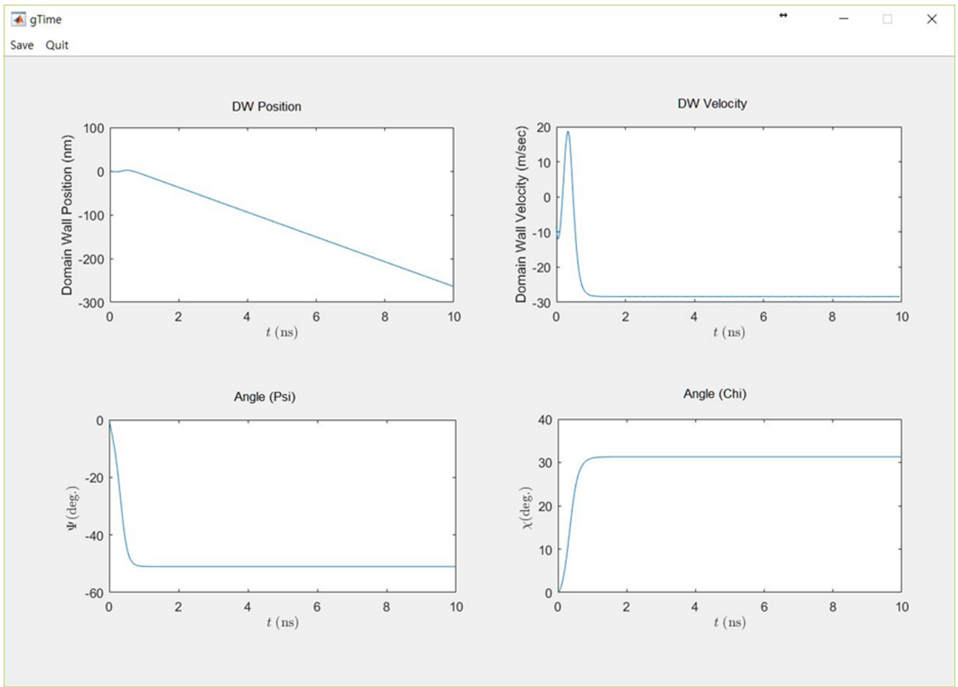

FIG. 3. The output dialog box showing DW position, DW velocity, DW angle, and DW tilting angle as a function of time, respectively.

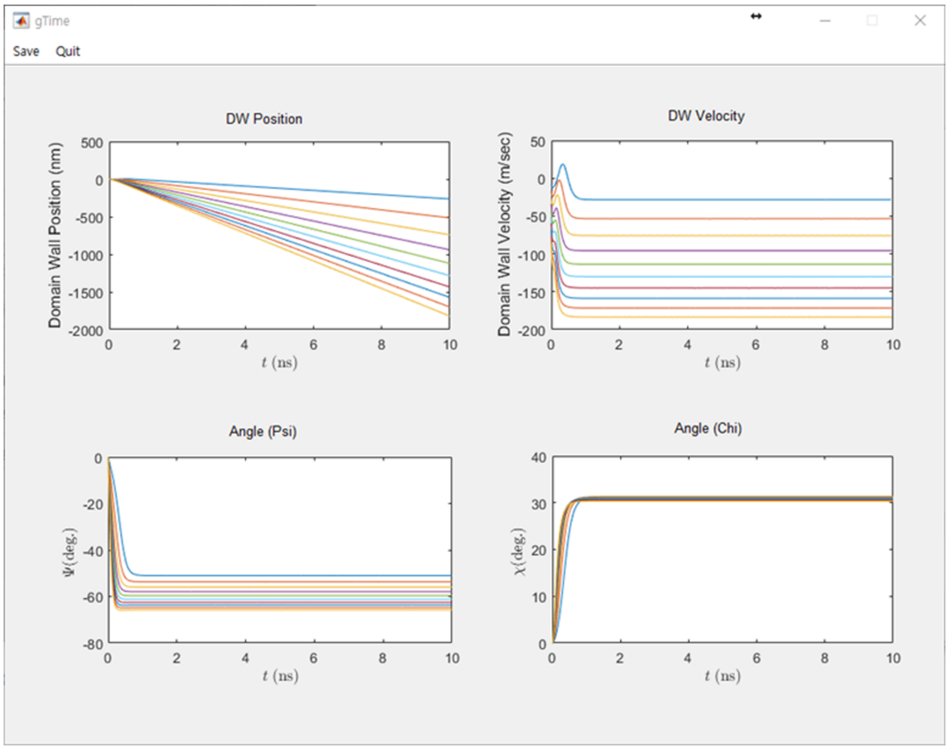

FIG. 4. The output dialog box with various increasing current densities. Calculated results for each current density are plotted together.

as shown in Fig. 4. In this case, we can easily obtain DW velocity as a function of the current density as shown in Fig. 5. We can also save these results. Here, it must be mentioned that the DW velocity plot in Fig. 5 is a collection of the last velocity value for a given current density. It is not an average velocity of DW. When DW motion involves precession, the plot may give misleading results. DW velocity plot may give improper results. More details will be explained in the next section. Use of this simulator is very straightforward and easy.

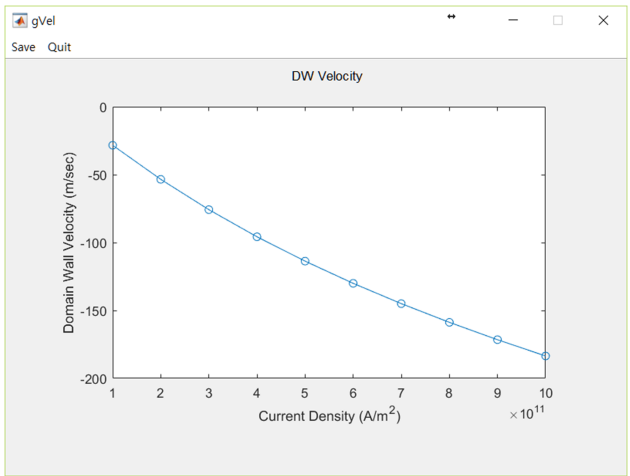

FIG. 5. DW velocity vs. current density for multiple current densities. One can save DW velocity as a function of current density.

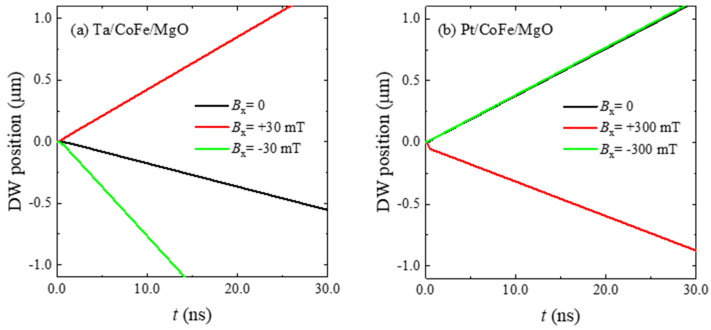

FIG. 6. DW positions for cases considered in Ref. 19. Results of our simulator are identical to Fig. 5 (a) and 5(c) of Ref. 19.

IV. SIMULATION RESULTS

In order to confirm the validity of the simulator, we reproduced results of Ref. 19 with the same materials parameters and simulation conditions. For CoFe, we used M_s = 7x10^{5}A/m, A_{ex} = 10 pJ/m, L_z = 0.6 nm, L_y = 160 nm, and K_u = 4.8x10^5 J/m^2. For Ta/CoFe/MgO (Pt/CoFe/MgO) case, D = -0.05 (-1.2) mJ/m^2, θ_{SH} = -0.11 (+0.07), and α = 0.03 (0.3), where D, θ_{SH}, and α values were determined by a combination of heavy and ferromagnetic layers. We ignored α_R and spin transfer torque effect in the test run. Therefore, we set P = 0.

Results for Ta/CoFe/MgO (B_x = 0, +30, and -30 mT) and Pt/CoFe/MgO (B_x = 0, +300, and -300 mT) corresponding to Fig. 5(a) and Fig. 5(c) of Ref. 19, respectively, are shown in Fig. 6(a) and 6(b). Their agreements are perfect.

When the current or field is small (the "flow region") the DW moves with constant angle Φ. When the field or current is larger than critical value (Walker breakdown), the DW moves by rotating tilting angle. This is the so-called precession region. When DW motion belongs to the precession motion region, there is a minor problem in the determination of DW velocity in this simulator. We calculated the DW velocity from the time derivative of DW displacement. This might have caused improper results in the DW velocity plot in the case of precession region. For example, if the DW motion belongs to the precession region, DW motion is more complicated over Walker breakdown. It seems that DW is moving forward in a large time scale (see Fig. 7(a)). However, details of DW motion are different as shown in Fig. 7(b). Φ is continuously rotating (increasing) while DW position is moving forward and backward with different amplitudes. Therefore, DW velocity by time derivative gives Fig. 7(c), oscillating with different sign. However, true velocity must be time average of the oscillating one or it can be simply obtained from slopes shown of Fig. 7(a), 2500 nm/10 ns ~ 250 m/s. In the simulator, we only provided oscillating velocity. Therefore, extra caution is required when one

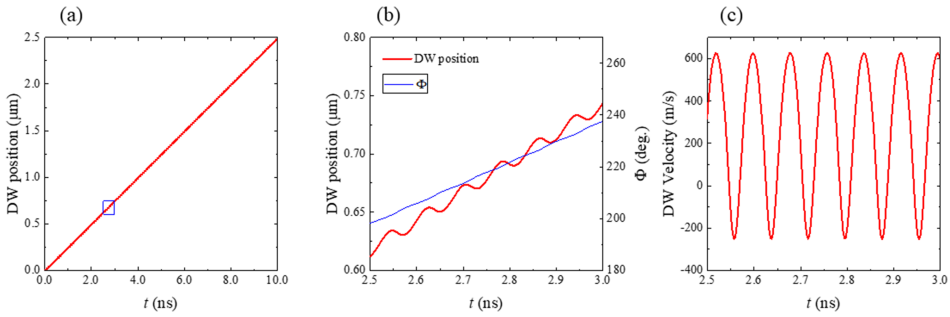

FIG. 7. (a) DW position as a function of time for precession DW motion. The blue rectangle indicates the range of plot (b). (b) Zooming of plot (a) for DW position and DW angle Φ, the forward and backward motion of DW. It clearly shows the trend of continuous increasing of Φ. (c) DW velocity calculated from the time derivative of DW position. It is oscillating, changing its sign. However, time averages are finite non-zero velocity values.

extracts DW velocity data for precession region of DW motion. As a result, for the case of multiple current densities, the final DW velocity plot (see Fig. 5) also provided improper results. Therefore, for simulation results of the DW velocity, users should determine whether DW motion belongs to the precession region.

V. CONCLUSIONS

We implemented a standalone DW simulator working with MATLAB library for one-dimensional DW motion based on the collective coordinate approach. The implemented simulator can calculate DW position, DW velocity, Φ (internal magnetization angle), and χ (DW tilting angle). We believe that the present simulator is useful for many experimentalists and help the obtain clear and transparent physical insights of DW dynamics under external magnetic field, spin transfer torque, and spin orbit torques (spin Hall, Rashba, and DMI).

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