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# Atomistic Modelling of Spatially Resolved Oscillation Dynamics in Ferrimagnetic Spin-Chain

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**Abstract**

**The dynamics of inhomogeneous spin textures in ferrimagnetic systems, such as domain walls and magnons, remain incompletely understood. To address this issue, we developed an atomistic model and observed spatially inhomogeneous THz-oscillation dynamics in a ferrimagnetic spin-chain. Our findings reveal that when excited by spin transfer torque, the spin-chain oscillates in the exchange mode with an inhomogeneous profile. Additionally, we propose an anti-parallel exchange length to quantify this inhomogeneity. This work provides new insights into ferrimagnetic spintronics and could help accelerate the development of new technologies that harness the unique properties of ferrimagnetic materials.**

## 1. Introduction

Ferrimagnets (FiMs) possess versatile properties due to their antiferromagnetic sublattice coupling and finite net magnetization. Research on FiMs highlights ultrafast dynamics, indicating a promising platform for information processing. However, current theoretical studies on the FiM dynamics typically treat the system as colinearly coupled sublattices or use the two-sublattice macro-spin model, coupling two Landau-Lifshitz-Gilbert-Slonczewski (LLGS) equations to describe the magnetization evolution.[1] Although these modeling contributed to our understanding of spin dynamics in FiMs, they fail to capture non-uniform spin textures, such as magnons and skyrmions, as well as exotic dynamics observed in recent experiments, such as asynchronous domain wall motion between different sublattices.[2]

Therefore, it is desirable to adopt a more accurate model that can simultaneously describe both individual and conjoint spin dynamics to investigate the asynchronous and inhomogeneous spin dynamics in FiMs. Additionally, spin-chains have proven to be instrumental in studying far-reaching spin dynamics, as demonstrated in previous research.[3] Recent advancements in techniques based on scanning tunneling microscopes and in-situ material synthesis have allowed us to engineer spin-chains on the ultimate atomic scale.

In this work, we investigate the oscillation dynamics induced by the spin transfer torque (STT) in a designed FiM spin chain using an atomistic model. Our findings reveal that when excited by STT, the spin chain oscillates in the exchange mode and exhibits an inhomogeneous profile. We propose an anti-parallel exchange length ($l_{AEX}$) to quantitatively describe the inhomogeneity. The analytical results of the $l_{AEX}$ are consistent well with the numerical results and reveal that the stronger AFM-like exchange coupling and smaller saturation magnetization of the host material result in the more remarkable inhomogeneity in the spin-chain. Notably, our atomistic model facilitates the observation of the inhomogeneous oscillation properties, which cannot be described using the two-sublattice macro-spin model.

## 2. Methodology

The atomistic model is illustrated in Fig. 1(a), where one down-spin from Gd atom is at the center of the spin-chain and denoted as "0". The rest include 100 up-spins from FeCo atoms and every spin is denoted. The FiM chain is then injected with spin-polarized electrons that exert STT to every atom. The magnetization dynamics of the FiM spin-chain is described by the coupled LLGS equations as follows: $d\boldsymbol{m}_i/dt = -\gamma_i \times \boldsymbol{H_{eff}} + \alpha \boldsymbol{m}_i \times d\boldsymbol{m}_i/dt - \gamma_i \boldsymbol{m}_i \times (m_i \times \boldsymbol{P_{STT}})$, where $i$ denotes the individual spins positioned at the atom side $i$. The effective field ($\boldsymbol{H_{eff}}$) is extracted from the Hamiltonian $\mathcal{H} = J_{ex} \sum_i \boldsymbol{m}_i \cdot \boldsymbol{m}_{i+1} - K_u \sum_i (\boldsymbol{m}_i \cdot \hat{\boldsymbol{z}})^2$, including the exchange interaction ($H_{ex}$) and the uniaxial anisotropy ($H_{ani}$). The last term in the LLGS equation represents STT-induced damping-like torque, where $\boldsymbol{P_{STT}}$ is the spin polarization.

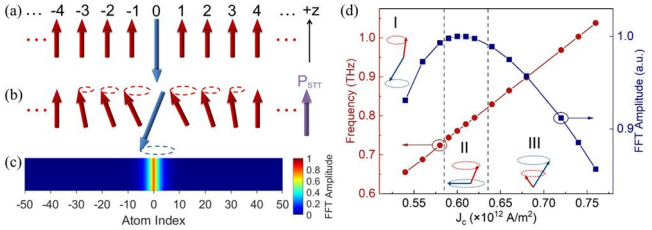


**Fig. 1.** Schematic of (a) the multi-spin model which describes the spin chain with 101 spins and (b) the oscillation profile excited by STT; (c) FFT amplitude distribution in the spin chain operated by $J_c = 0.7 \times 10^{12}\ A/m^2$. (d) Frequency and FFT amplitude as a function of $J_c$.

## 3. Results and Discussion

As shown in Fig. 1(b), when injected electrons with the $\boldsymbol{P_{STT}}$ parallel to the +z axis, only some specific spins, which locate close to the opposite-spin spatial region, formed stable oscillation in the exchange mode. While the rest of spins are stabilized by the $\boldsymbol{P_{STT}}$ and keep static. We define the opposite-spin spatial region as "oscillation core (OC)", in that the oscillation stems from the antiferromagnetic exchange interaction in this region. The oscillation amplitude distribution shown in Fig. 1(c) indicates that although we only consider nearest neighbor exchange interaction, the anti-parallel exchange interaction (AEI) can indirectly influence the spins near the OC (corresponding to the atom with index 2, 3 and so on), resulting in the stable oscillation. Beyond the indirect influence range, the spins keep static. The spatially inhomogeneous oscillation profile observed in the ferrimagnetic

spin-chain will be discussed in detail later. Additionally, due to the strong exchange coupling, the spins in the stable oscillation state share the same frequency and exhibit three typical phases, as shown in Fig. 1(d).

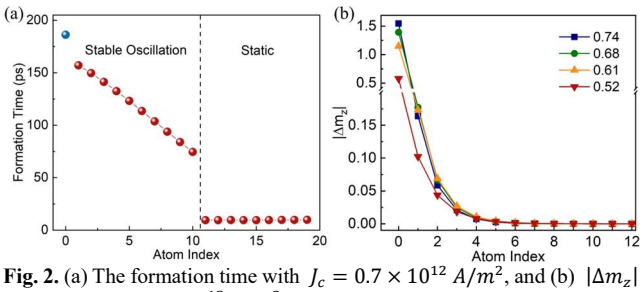


**Fig. 2.** (a) The formation time with $J_c = 0.7 \times 10^{12}\ A/m^2$, and (b) $|\Delta m_z|$ with different $J_c$ ($\times 10^{12}\ A/m^2$) as a function of atom index.

The amplitude distribution and identical frequency indicate that the spin closer to the OC exhibits a larger linear velocity and thus requires more time to form stable oscillation, whereas the rest of spins keep static, as demonstrated in Fig. 2(a). To qualitatively investigate the inhomogeneous profile, the amplitude distribution is further evaluated. The oscillation amplitude relates to the variation of the $\hat{z}$ component of the $\boldsymbol{m}$ ($|\Delta m_z|$), and the $|\Delta m_z|$ implies the atoms that form stable oscillation ($|\Delta m_z| \neq 0$) or relax to the z-axis and remain static ($|\Delta m_z| = 0$). Interestingly, it can be observed that the number of oscillatory atoms remains constant even when operated at different $J_c$, as shown in Fig. 2(b).

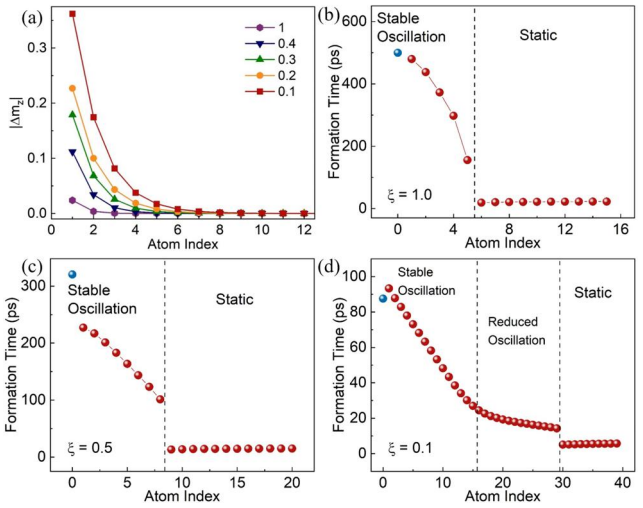


**Fig. 3.** (a) $|\Delta m_z|$ as a function of atom index with different ξ. The formation time with respect to spatial position in the FiM spin chain with (b) ξ = 1.0; (c) ξ = 0.5; and (d) ξ = 0.1.

Furthermore, by analyzing $|\Delta m_z|$ shown in Fig. 3(a), it was determined that the number of atoms that can be facilitated in a stable oscillation state depends on ξ, which represents the ratio of individual spin angular momenta of the opposite spins (here we fix the magnetic moment of Gd and change the magnetic moment of FeCo). Smaller ξ facilitates more atoms to oscillate due to more remarkable AEI. Besides, Fig. 3(b) and (c) show that the spin chain with reduced ξ requires less time to form stable oscillation and exhibits a stable oscillatory phase within the range affected by the AEI. When ξ is further reduced, the dynamic phase involves into a stable oscillation and a decaying oscillation, indicating that the effect of AEI still exists but is not strong enough to maintain the stable oscillation, as shown in Fig. 3(d).

The inhomogeneous oscillation induced by the AEI can be understood quantitatively by the competition between the $H_{ex}$ and the $H_{ani}$. The internal Bloch structure, in principle, shares a similar physics principle to the Bloch domain wall, whose width can be described by the exchange length $l_{EX} = \sqrt{A_{EX}/K_u}$. Hence, we calculate an $l_{AEX}$ expressed as:

$$l_{AEX} = \sqrt{|J_{A-B}|/(a\mu_0 M_{s,A}^2)}$$

The $J_{A-B}$ is the anti-parallel exchange factor, wherein A (B) is for the atom of the host material (doped material). For the spin chain, the number of atoms within the $l_{AEX}$ can be calculated as $N = l_{AEX}/a$, where $a$ is the lattice constant.

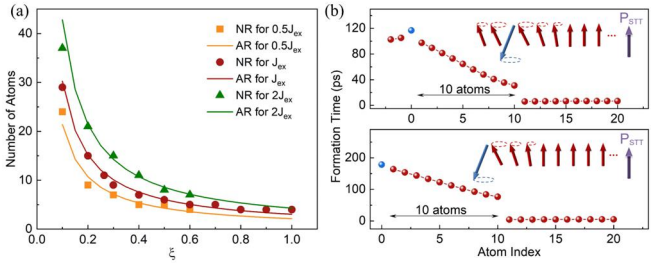


**Fig. 4.** (a) Comparation between the NR and AR of the number of atoms within the $l_{AEX}$; (b) The $l_{AEX}$ of the different position of the OC.

To verify the analytical solution of the $l_{AEX}$, we not only investigate the spin chain composed of GdFeCo, but also change the value of $J_{A-B}$ for the parametric study. As shown in Fig. 4(a), the analytical results (AR) are consistent with the numerical results (NR), and reveal that the larger $J_{A-B}$ or smaller $M_s$ of the host material would result in longer $l_{AEX}$. Additionally, we find that the $l_{AEX}$ is independent of the position of the OC as shown Fig. 4(b).

## 4. Conclusion

In summary, we investigated the inhomogeneous oscillation dynamics in the FiM spin-chain through qualitative and quantitative analysis using the atomistic model. An anti-parallel exchange length is implemented to quantitatively analyze the inhomogeneity arising from the AFM-like exchange interaction. The results reveal that the inhomogeneity can be enhanced by the stronger AFM-like exchange coupling and smaller saturation magnetization of the host material. Our work provides insights into the FiM spin dynamics and can guide the design of materials for ultrafast spin nano oscillators.


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**Reference:**


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