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Spontaneous creation and annihilation dynamics of magnetic Skyrmions at elevated temperature

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Skyrmions are topologically protected nanoscale magnetic structures with a wide range of potential applications. Here we determine the life cycle of Skyrmions from their creation, to their intrinsic dynamics and thermal stability to their eventual thermodynamic demise. Using atomistic simulations of Ir/Co/Pt, parameterized from *ab-initio* calculations, we demonstrate the thermal phase transition to a Skyrmion state under application of a perpendicular magnetic field. The created Skyrmions exhibit Brownian particle-like dynamics driven by the underlying thermal spin fluctuations. At an elevated temperature window well below the Curie temperature, the Skyrmions are metastable and can collapse to a uniform magnetic state. With application of an external magnetic field, the intrinsic local thermal spin fluctuations at this elevated temperature window are sufficiently large to allow the spontaneous formation of new Skyrmions in thermodynamic equilibrium analogous to a spontaneous Skyrmion gas. Such a system could be used to implement a Skyrmion based true random number generator.

I. INTRODUCTION

The magnetic Skyrmion is a topological nontrivial magnetisation configuration, shown to be found in magnetic materials which exhibit antisymmetric exchange, also known as the Dzyaloshinskii-Moriya interaction (DMI) [1–5]. The DMI relies on spin orbit coupling, which usually is provided by the heavy metal layer in the system [6]. Skyrmions can be used as building blocks in the development of next generation logic and data storage devices. In comparison with domain walls, Skyrmions represent better candidates for potential applications due to the lower critical current threshold (10^6 A/m²) to move them [7–9]. In nanoscale devices, Skyrmion motion can be driven via spin polarised currents, spin waves and temperature gradients [10–13]. During the displacement of magnetic Skyrmions driven by a current or gradient in the nanoscale device, the Magnus force on the Skyrmion causes it to move toward the edge, a phenomenon known as the Skyrmion Hall Effect (SkHE) [14]. Magnetic Skyrmion based devices are suggested for future data storage device applications. However, thermal effects arising from the environment or spin polarized currents affect the practical application of magnetic Skyrmion based spintronic devices [15–18].

Thermal activation has usually been considered detrimental to magnetic Skyrmions due to its potential to bypass their topological protection, thus being able to irreversibly deform or switch the chiral structures. Previous results have shown that Skyrmions can be created by Joule heating and temperature gradients present in the device [17, 19], but there is little published information on the behaviour of magnetic Skyrmions under strong thermal effects. The study of thermal

effects in Skyrmions can provide guidelines to room temperature Skyrmion based devices [20–23] and give further insights on the generation mechanisms of Skyrmions via temperature pulses that have been observed both by calculations and experiments [19, 24, 25]. Furthermore, the thermally induced Skyrmion creation/annihilation and Skyrmion dynamics show their potential as true random seed generators and provide insight on Skyrmion transport under elevated temperature conditions [26–30]. It is necessary to develop suitable models to study Skyrmion dynamics at elevated temperatures. At the moment, there are models based on Micromagnetic simulations mainly [27, 28], however atomistic simulation with the full range of exchange interactions from *ab-initio* calculations [30, 31, 43] is an important model to investigate Skyrmion behavior at high temperatures. Atomistic simulations can model the time evolution of the spin configurations of Skyrmion based devices at elevated temperature, and explain how the thermal effect affects device performance.

In this Letter, we use atomistic spin dynamics simulations with *ab initio* parameterization to investigate Skyrmion dynamics at elevated temperatures well below the Curie temperature (T_c). The elevated temperature in this work is taken from 300 K ($0.461 T_c$) to 500 K ($0.769 T_c$). The results in this work present a time-resolution dynamics of skyrmion creation and annihilation in magnetic chiral thin films under strong thermal effect. The simulation results reveal thermally induced phase transitions between the Skyrmion, stripe domain and ferromagnetic states. We explore the behaviour of the ferromagnetic and stripe domain states under different thermal processes as well as the required conditions for Skyrmion creation and annihilation. Our results show that

even at temperatures below the Curie temperature, it is possible to spontaneously generate a Skyrmion in the thin film through a purely intrinsic thermal effect, circumventing their assumed feature of being topologically protected structures.

II. MODELING AND SIMULATION

The simulations have been performed using the atomistic spin dynamics software package VAMPIRE 5.0 [33]. The model is based on the parameters from *ab-initio* calculations and includes the full range of exchange interactions of the FCC Ir/Co/Pt system. Self-consistent calculations were performed for a model multilayer of 3Co/3Ir/3Co/3Pt/3Co layers sandwiched from both sides by Pt(111) by using the Screened Korringa-Kohn-Rostoker method [34, 35]. The electronic structure was determined in the paramagnetic state in terms of the scalar-relativistic disordered local moment (DLM) approach [36], while the spin-cluster expansion technique as combined with the relativistic DLM technique [37] was employed to derive tensorial exchange interactions. The spin Hamiltonian \mathcal{H} of the system is described by an extended Heisenberg spin model with the following form:

$$\mathcal{H} = - \sum_{i < j} (\mathbf{S}_i \mathcal{J}_{ij} \mathbf{S}_j) - k_u \sum_i (\mathbf{S}_i \cdot \mathbf{e})^2 - \sum_i \mu_i (\mathbf{S}_i \cdot \mathbf{B}_{app}) \quad (1)$$

where $\mathbf{S}_i, \mathbf{S}_j$ are the normalised spin vectors on i, j sites, \mathcal{J}_{ij} is the exchange matrix calculated *ab-initio*, k_u is the uniaxial magnetocrystalline anisotropy energy (MAE) constant per site, μ_i is the atomic spin moment, \mathbf{B}_{app}

is the external field. The *ab-initio* exchange matrix is defined below, where the off-diagonal parts of the matrix represent the DMI vector components, D_{ij} :

$$\mathcal{J}_{ij} = \begin{bmatrix} J_{xx} & J_{xy} & J_{xz} \\ J_{yx} & J_{yy} & J_{yz} \\ J_{zx} & J_{zy} & J_{zz} \end{bmatrix}_{ij} = \begin{bmatrix} J_{xx} & J_{xy}^S + D_z & J_{xz}^S - D_y \\ J_{xy}^S - D_z & J_{yy} & J_{yz}^S + D_x \\ J_{xz}^S + D_y & J_{yz}^S - D_x & J_{zz} \end{bmatrix}_{ij} \quad (2)$$

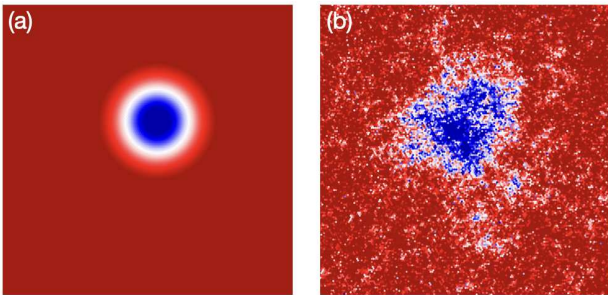


FIG. 1. Thin film spin configurations of an isolated Skyrmion at different temperatures: (a) 0 K Skyrmion ground state (b) 300 K room temperature Skyrmion deformation. The colour palette is determined by the M_z (red for +1, white for 0 and blue for -1)

The model considers finite temperature via the introduction of the stochastic field into the effective field in the atomistic Landau–Lifshitz–Gilbert equation [38]. Within this approach, the stochastic field is introduced as a white noise term, its properties being in agreement with the fluctuation-dissipation theorem and correctly leading to the Boltzmann equilibrium distribution [39–41]. The accuracy of the results is assured by a integration timestep of $5 \cdot 10^{-16}$ s. In this work, we explicitly include in our atomistic model only the three Cobalt layers between the Ir and Pt. The parameters for the atomistic spin model are given in the Supplemental Material [42]. The Skyrmion number in this work is calculated from the topological charge [43, 44].

III. RESULTS AND DISCUSSION

There are three magnetic phases in the Ir/Co/Pt multilayer system: the ferromagnetic phase, the stripe domain phase and the Skyrmion phase which has also been found in other systems [2, 45]. Skyrmion simulations at elevated temperatures also show the thermally induced phase transition between these three phases. The initial spin configurations are given in Fig. S3 in the Supplemental Material [42]. The system size is $30 \text{ nm} \times 30 \text{ nm} \times 0.25 \text{ nm}$, with periodic boundary conditions in the x and y directions. The ferromagnetic and the stripe domain configurations are obtained by relaxing the system at 0 K in zero applied field, while the Skyrmion phase is obtained in a 1 T field relaxation process. When the temperature is higher than 100 K, the stripe domain will be generated by the thermal effect, the mean-magnetisation-length will drop to near 0, which means the ferromagnetic state is no longer the ground state of the system.

The ground state Skyrmion phase and the same structure visualised at an elevated temperature is shown in Fig. 1. The diameter of the Skyrmion is around 5 nm at 0 K, while thermal noise leads to a significant distortion of the Skyrmion structure although the characteristic size is not significantly different.

We first consider the stripe domain phase under high temperature conditions (300 K to 500 K). The simulation time has been set to 10 ns which is long enough to give a clear diagram of the phase transition in the system. The initial state for the spin configuration is given in Fig. S3(c). The stripe domain state can be stable without external field at 0 K. The 10 ns simulation of the stripe domain state for different temperatures is given in Fig. 2. Here thermal effects distort the shape of the stripe domains and we define a critical temperature at which the stripe domains undergo a phase transition. Below this threshold temperature the spin texture diffuses due to the thermal fluctuations but its overall morphology is unchanged. Above the critical point, the system displays a thermally induced stripe-domain bending. This effect generates a hybrid magnetic configuration in which both Skyrmions and stripe domains can be found. The result from Fig. 2 to Fig. 4 is averaged from 10 spin configurations in the same time range, in order to avoid large fluctuations from the strong thermal noise

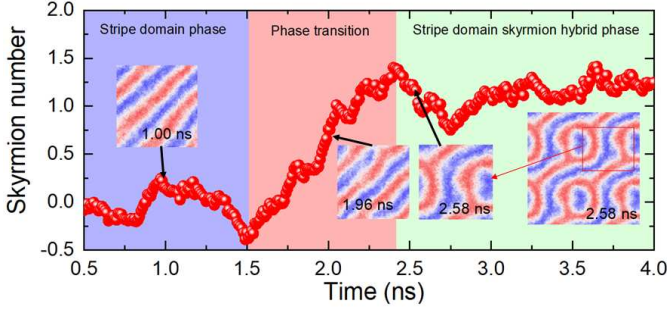


FIG. 2. The spin configuration of the stripe domain broken at 450 K. The system displays an initial stripe domain phase followed by a transition towards a hybrid stripe domain-Skyrmion phase.

and give a better representation of the phase change.

Fig. 2 further investigates this behaviour, highlighting the time-evolution of the striped texture at a temperature of 450 K. During the first 1.5 ns, it can be seen how the thermally-induced diffusion process alters the magnetic configuration. Gradually moving our perspective in time, we find a bending and shrinking of the stripe-domains, which eventually leads to Skyrmion nucleation in agreement with a Skyrmion number of 1 and the aforementioned hybrid phase. As given in Fig. S4 in the Supplemental Material [42], the ground state of the system is the stripe domain state in absence of an external field. When a 1 T external field is applied to the system, the ground state is the skyrmion state. Simulations of the stripe domain phase with different random seeds are given in section 5 of the Supplemental Material [42], showing that the final state of the system is dependent on the random thermal fluctuations. From the results in section 5 of the Supplemental Material [42], the possibility of $S_n = +1$ Skyrmion creation and $S_n = -1$ Skyrmion creation in the system is the same which suggests that these processes are equivalent in a defect free system.

When an external field is applied to the system, the Skyrmion state becomes the ground state of the system. For this state at elevated temperatures the system goes beyond distortion of the spin texture into a region of spontaneous Skyrmion creation and annihilation. Fig. 3 demonstrates the creation and annihilation process for a system at $T = 500$ K in an applied field of 1 T. The initial spin configuration for Fig. 3 is a Skyrmion which is given in Fig. S3(b) in the Supplemental Material [42]. According to the spin configuration in Fig. 3, spins fluctuate in the system and spin flip events generate a spin texture which is stabilised by the DMI. To here, the DMI in the system protects the spin texture from thermal effects and the external field, and the spins are twisted around the nucleus of a magnetic Skyrmion. From Fig. 3 (a), a second Skyrmion first generated by the thermal field grows to the same size as the original Skyrmion. The size of the Skyrmion is determined by the balance between exchange interaction, DMI and magnetic anisotropy and their temperature dependence. Evidence for the annihilation of a magnetic Skyrmion

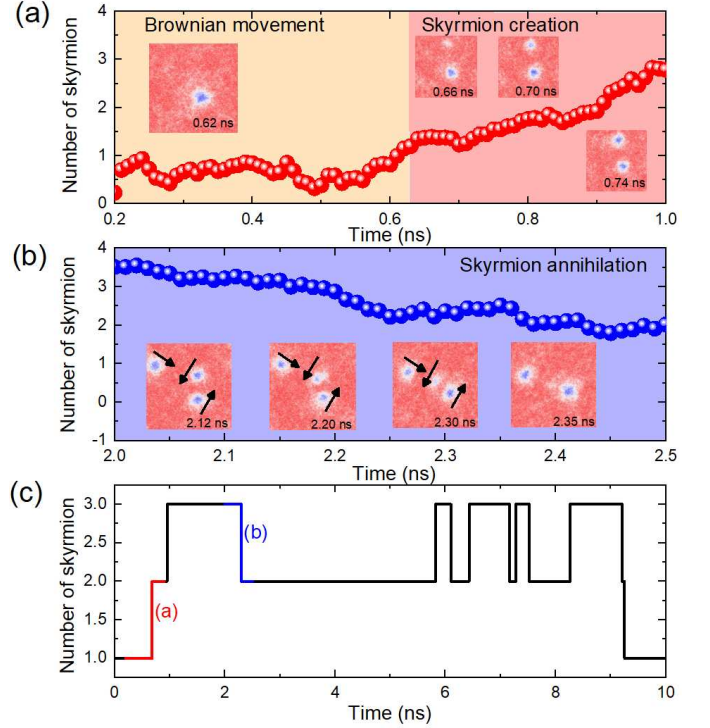


FIG. 3. (a) The spin configurations and Skyrmion number during the Skyrmion creation in the system. (b) The spin configurations and Skyrmion number during Skyrmion annihilation in the system. The spin configuration for Skyrmion nucleated in the system at 500 K. The trend of the Brownian motion of Skyrmion has been marked as black arrows. (c) Time dependence number of magnetic Skyrmion under a 500 K thermal condition where (a) and (b) refer to figure panels respectively. The number of magnetic Skyrmion is comes from the averaged spin configuration.

is given in Fig. 3(b). At this stage in the time evolution of the Skyrmion state, a third Skyrmion has been thermally created. Under the thermal effect, magnetic Skyrmions exhibit a breathing mode, with diameters increasing and decreasing due to the thermal activation. The fluctuations lead to deformation of the Skyrmion which can destroy its topological protection. As evidence, from Fig. 3(b), the size of one particular Skyrmion begins to decrease and then the Skyrmion disappears from the system. From the simulation results in Fig. 3, the thermal creation and annihilation of magnetic Skyrmions is clear. Furthermore, the Skyrmions are easier to create by thermal fluctuations at higher temperatures and also the lifetime of Skyrmions will be decreased. This is a statistical thermodynamic process and is subjected to fluctuations, but these initial results point to creation and annihilation of Skyrmions at elevated temperatures. To account for the stochastic nature of thermal effects, the evolution of the system from a defined magnetic state under 10 different pseudo-random number seeds is investigated and shown in the Section 6 of the Supplemental Material [42]. t_{start} is the time at which the initial magnetic configuration from which the simulations are restarted with different seeds is taken. From the simulation re-

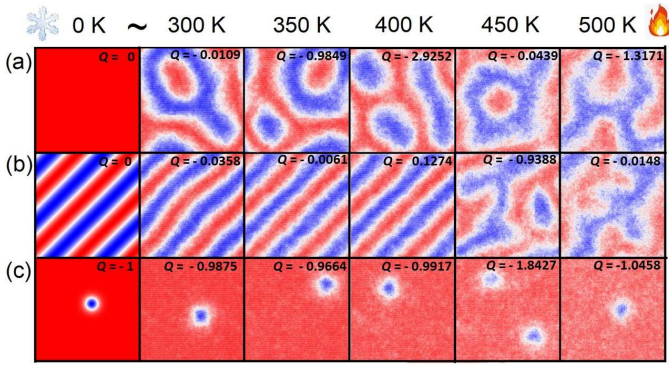


FIG. 4. The transition between the three states in the Ir/Co/Pt system. (For the 10 ns simulation) (a) The phase between the Ferromagnetic phase and Skymion+Stripe domain state. (b) The transition between the Stripe and Skymion+Stripe domain state. (c) The transition between the Skymion state and Skymion creation/annihilation state.

sults presented in Fig. S6(a), when the initial state is taken at $t_{start} = 0.30$ ns, different random fields yield a large variety of final states that range from Skymion number 0.5 to 2.5. On the other hand, for $t_{start} = 0.35$ ns the system seems to evolve towards the creation of an extra Skymion, with Skymion number 2. These results show that the Skymion state, which is stabilised by DMI, can persist under thermal effects.

From the simulation results in Fig. 4 (c), the Skymion is stable and diffusive in the system due to the thermal effect. In the final state for the Skymion at $T = 450$ K, the image shows two Skymions in the system which means that at temperature greater than around 400 K, spontaneous thermal creation of Skymions can occur. The calculated time dependence of the Skymion number for temperatures from 450 K to 500 K is shown in the section 7 of the Supplemental Material [42] with a Skymion number for the initial as 1. The observed time dependence of the Skymion number is indicative of the creation and annihilation of Skymions at elevated temperatures. The data show large variations over temperature because of the small system size, although a trend towards larger Skymion numbers and more rapid creation and annihilation can be seen. Particularly, for the 500 K case, the Skymion number is changing especially rapidly. Generation and destruction of Skymions over time are shown in Fig. 3(a) (0.6 ns to 0.8 ns) and Fig. 3(b) (2.1 ns to 2.4 ns). The time dependence of the number of magnetic Skymions is given in Fig. 3(c). For temperatures of $T = 500$ K the spontaneous creation and annihilation of Skymions at nanosecond timescales represents a 2D Skymion gas with a statistically varying number of particles that may be an interesting physical system to explore. The total energy of the system in ferromagnetic state and skymion state at 0 K with a 1T external field is given in the section 8 of the Supplemental Material [42].

The transition between different magnetic states in the Ir/Co/Pt system has been demonstrated by the simulation results and is presented in in Fig. 4. For an initial ferromagnetic state, which is not the ground state of the system, the

system experiences a transition towards a stripe domains state due to thermal effects. Upon further temperature increases, the system transitions to the Skymion/stripe domain hybrid state. When the initial state of the system is the stripe domain state, with the temperature above 450 K, the stripe domain is perturbed by the thermal field and the system evolves to the Skymion/Stripe domain hybrid phase. This is similar to the case of the initial ferromagnetic state. When the simulation is set to start from a Skymion state, this seem to remain stable up to 400 K. For temperatures greater than 450 K, thermal creation of Skymions in the system occurs. If the temperature continues to increase around 500 K, the Skymion may be destroyed by the thermal fluctuations and transition to a Skymion creation/annihilation state.

IV. CONCLUSION

In conclusion, we have studied the magnetic phases of the Ir/Co/Pt system via an atomistic spin model. The model is based on parameters from the ab-initio calculations and includes the full range of exchange interactions of the system. Our results show that if temperature increases, the mean Skymion lifetime reduces and there is a larger probability of the spontaneous thermal creation/annihilation of Skymions. Our atomistic simulations have demonstrated that the thermal Skymion creation could occur at a temperature window much lower than the system Curie temperature. The transitions towards chiral material-systems is well explained by our model which is important for advanced Skymion based spintronic devices. For example, Skymions randomly created by thermal effects could be used as true random number generators in a computing device.

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