Monte Carlo studies on shape deformation and stability of 3D skyrmions under mechanical stresses

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Abstract. We study the stability/instability of skyrmions under mechanical stresses by Monte Carlo simulations in a 3D disk composed of tetrahedrons. Skyrmions emerge in chiral magnetic materials, such as FeGe and MnSi, under the competition of ferromagnetic interaction (FMI) and Dzyaloshinskii-Moriya interaction (DMI) and are stabilized by the external magnetic field. Recent experimental studies show that skyrmions are also stabilized/destabilized by uniaxial compressive stress perpendicular to or along the magnetic field direction. These phenomena are studied by using a 3D Finsler geometry (FG) model. In this 3D FG model, the DMI coefficient is automatically anisotropic by a geometrically implemented coupling of strains and electronic spins. We find that skyrmions are stabilized (destabilized) by extension (compression) stress along the direction of the applied magnetic field consistent with reported experimental data. This consistency implies that the 3D FG model successfully implements the magnetostrictive or magneto-elastic effect of external mechanical stresses on chiral magnetic orders, including the skyrmion configuration.

1. Introduction
Skrymions are topologically stable spin configurations in chiral magnets and attract much attention for their potential in spintronics devices [1]. Recent experimental studies have indicated that mechanical stresses play a non-trivial role in deforming skyrmion configurations, and the skyrmion shape deforms under uniaxial tensile stress perpendicular to the magnetic field [2, 3]. Skyrmions are also stabilized/destabilized depending on whether the stress is tensile or compressible along the applied magnetic field direction [4, 5]. As a consequence, the area of the skyrmion pocket in the $BT$ phase diagram, where $B$ is magnetic field and $T$ the temperature, shrinks/expands depending on the stress direction.

The authors recently studied skyrmion deformation by Monte Carlo simulations on 2D triangular lattices and concluded that the shape deformation can be attributed to anisotropy in the Dzyaloshinskii-Moriya interaction (DMI) [6]. In this study, we extend this model to a 3D model on tetrahedral lattices of thin disk. We expect that the same conclusion will be
obtained in the 3D model for skyrmion deformation such that the DMI anisotropy is the origin of deformation. As it turned out, the DMI anisotropy is found in this work to be also the origin of deformation. Moreover, we find that the DMI anisotropy in the 3D model can give rise to the stabilization/destabilization of skyrmions. So, we conclude that the 3D FG model introduces a magneto-elastic effect responsible for the stabilization/destabilization of skyrmions.

2. Model
First, we show snapshots of 3D skyrmions in the 3D disk composed of tetrahedrons. Figure 1(a) is an upside view and Fig. 1(b) shows spins of $\sigma_z \geq 0$ with the side and lower surfaces of the 3D disk, where spins of $\sigma_z < 0$ and tetrahedron lattices are eliminated. These skyrmions are in a vacuum (or ground state) configuration.

Figure 1: Snapshots of skyrmion vacuum configuration in (a) 2D and (b) 3D visualizations. The 3D disk is composed of tetrahedrons like in (c), and the total number $n_{ij}$ of tetrahedrons that share the bond $ij$, shown in (d) is not uniform in this 3D disk.

To implement magnetoelastic effects in the model, we assume a non-polar internal strain field $\tau$ of unit length. The direction of $\tau$ is defined such that $\tau$ is parallel to the direction along which the distance between two atoms increases. This definition of $\tau$ is well-defined for tensile forces in both 2 and 3 dimensions (Figs. 2(a), (b)). However, the direction is well-defined for compression only in 2 dimensions. This implies that the 3D extension of the 2D skyrmion models in Ref. [6] is non-trivial and worth studying in detail.

Figure 2: Internal strain field directions under extension (solid arrow $\uparrow$) and compression (dashed arrow $\leftrightarrow$) in (a) 2D and (b) 3D. In the case of compression, the direction of strain field is uniquely (not always uniquely) determined in 2D (3D) materials.

The partition function is given by $Z = \sum_{\sigma} \exp(-S/k_BT)$, where $k_B$ and $T$ are the Boltzmann constant and the temperature, and $S$ is the discrete Hamiltonian given by

$$ S = \lambda S_{FM} - S_B + DS_{DM} + \gamma S_\tau - \alpha S_f, \quad (\alpha = 1). \quad (1) $$

Ferromagnetic interaction (FMI) and DMI energies $S_{FM}$ and $S_{DM}$, and other terms are given in Appendix A.

3. Results
Figures 3(a),(b) show snapshots of skyrmion shapes deformed and oblong along the tensile force directions $\mathbf{f} = (1, 0, 0)$ and $\mathbf{f} = (0, 1, 0)$. The shape is consistent with the experimental result in [2].
Figure 3: Snapshots of skyrmions under uniaxial tensile stress of (a) $\vec{f} = (1, 0, 0)$ and (b) $\vec{f} = (0, 1, 0)$. The skyrmion shape is oblong along the tensile stress direction and consistent with the experimental data in [2].

Figure 4: (a) A phase diagram of the model obtained under $\vec{f} = (0, 0, 0)$, and (b)–(g) snapshots in different phases. The horizontal and vertical axes represent the temperature $T$ and external magnetic field $B$, respectively. The solid symbols denote the three different phases, and the open symbols denote intermediate phases, some of which are expected to disappear after a sufficiently large number of MC iterations.

A $BT$ phase diagram for $\vec{f} = (0, 0, 0)$ and snapshots are shown in Figs. 4(a)–4(g). We have three different phases (ferromagnetic (ferro), skyrmion (sky) and stripe (stripe) phases) and the intermediate phases denoted by sk-fe, sk-st and st-fe between the three different phases. The paramagnetic (para) phase is expected in the region $B \to 0$ with sufficiently large $T$, however, the para is not detected in the region $T \simeq 3$.

Figure 5: (a) A phase diagram of the model obtained under pressure $\vec{f} = (0, 0, -5)$, and (b)–(g) snapshots in several different phases. The area of sky phase shrinks indicating that the skyrmion configuration is destabilized by uni-axial pressure along the direction of $\vec{B} = (0, 0, B)$. Figures 5(a)–5(g) are a phase diagram and snapshots corresponding to the uni-axial pressure $\vec{f} = (0, 0, -5)$ along the direction of $\vec{B} = (0, 0, B)$. We find that the area of the skyrmion pocket shrinks. This is consistent with the reported experimental results [4, 5].
4. Concluding Remarks
This paper studies 3D skyrmion shape deformation and stability/instability under mechanical stresses. In the 3D model, a realistic microscopic strain field can be introduced, leading to a proper interaction of strain and spins playing a role in the magneto-elastic effect on chiral magnetic orders, including skyrmions. The presented MC data are consistent with reported experimental results in that uniaxial pressures along the magnetic field direction destabilize skyrmion configurations. To get more detailed information on the magneto-elastic effect, we have to perform further MC simulations. Systematic computational tasks are yet to be completed.

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Appendix A

\[ S_{FM} = \sum_{ij} (1 - \sigma_i \cdot \sigma_j), \quad S_{DM} = \sum_{\Delta} \left( \sum_{ij(\Delta)} \Gamma_{ij} \vec{e}_{ij} \cdot \sigma_i \times \sigma_j \right), \]

\[ \Gamma_{ij} = \tilde{\Gamma}^{-1}_{n_{ij}}, \quad \tilde{\Gamma} = \sum_{\Delta} \sum_{ij(\Delta)} \frac{v_{ij}}{n_{ij}} \]

\[ S_B = \sum_i \sigma_i \cdot \vec{B}, \quad \vec{B} = (0, 0, B), \quad S_\tau = \frac{1}{2} \sum_{ij} (1 - 3(\tau_i \cdot \tau_j)^2), \]

\[ S_f = \text{sgn}(f) \sum_{\Delta} \left( \Gamma_{ij} \sigma_i \times \sigma_j \right), \quad \tilde{f} = (f_x, f_y, f_z), \quad \text{sgn}(f) = \begin{cases} 1 \text{ (tension)} \\ -1 \text{ (compression)} \end{cases} \]

where \( n_{ij} \) is the total number of tetrahedrons linked to the bond \( ij \) (Fig. 2(a)), \( \Gamma_{ij}^0 \) is a mean value of \( \Gamma_{ij} \) obtained with 1000 isotropic configurations of \( \tau \), and \( \Gamma_{ij} \) for a tetrahedron in Fig. 1(c) are given by

\[ \Gamma_{12} = \frac{v_{12}}{v_{12}v_{14} + v_{14}}, \quad \Gamma_{13} = \frac{v_{13}}{v_{13}v_{14} + v_{14}}, \quad \Gamma_{14} = \frac{v_{14}}{v_{14}v_{12} + v_{12}}, \quad \Gamma_{23} = \frac{v_{23}}{v_{23}v_{24} + v_{24}}, \quad \Gamma_{24} = \frac{v_{24}}{v_{24}v_{21} + v_{21}}, \quad \Gamma_{34} = \frac{v_{34}}{v_{34}v_{31} + v_{31}}, \quad \Gamma_{41} = \frac{v_{41}}{v_{41}v_{42} + v_{42}}, \]

where \( \vec{e}_{ij} \) is the unit tangential vector from the vertices \( i \) to \( j \), and \( v_0 \) is a cutoff. Here, \( \sum_\Delta \) and \( \sum_{ij(\Delta)} \) denote the sum over all tetrahedrons and sum over six bonds \( ij \) of tetrahedron \( \Delta \). From these definitions, we find that \( \sum_{\Delta(\bar{i})} \Gamma_{ij} \approx 1 \) for isotropic configuration of \( \tau \), where \( \sum_{\Delta(\bar{i})} \) is the sum over all tetrahedrons sharing bonds \( ij \) and \( \sum_{\Delta(\bar{i})} 1 = n_{ij} \) (Fig. 1(d)). \( S_B \) is the Zeeman energy and \( \vec{B} \) is the magnetic field. The energy \( S_\tau \) for \( \tau \) is the same as for liquid crystals, and \( \tilde{f}(\in \mathbb{R}^3) \) in \( S_f \) is the external mechanical force or stress. More detailed information on FG modeling and \( \Gamma_{ij} \) will be reported elsewhere.

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