Micromagnetic Simulations Study of Skyrmions in Magnetic FePt Nanoelements

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October 2, 2018

Abstract

The magnetization reversal in 330nm triangular prismatic magnetic nanoelements with variable magnetocrystalline anisotropy similar to that of partially chemically ordered FePt is studied using micromagnetic simulations employing Finite Element discretizations. Several magnetic properties including the evaluation of the magnetic skyrmion number $S$ are computed in order to characterize magnetic configurations exhibiting vortex-like formations. Magnetic vortices and skyrmions are revealed in different systems generated by the variation of the magnitude and relative orientation of the magnetocrystalline anisotropy direction, with respect to the normal to the triangular prism base. Micromagnetic configurations with skyrmion number greater than one have been detected for the case where magnetocrystalline anisotropy was normal to nanoelement’s base. For particular magnetocrystalline anisotropy values three distinct skyrmions are formed and persist for a range of external fields. The simulation-based calculations of the skyrmion number $S$ revealed that skyrmions can be created for magnetic nanoparticle systems lacking of chiral interactions such as Dzyaloshinsky-Moriya, but by only varying the magnetocrystalline anisotropy.

1 Introduction

Magnetic nanoparticles are vortex-like magnetization configurations. They have been predicted theoretically by Bogdanov et al. [3, 4] long before their experimental detection and discovery [26, 24]. In recent years magnetic skyrmions have attracted a lot of theoretical [13, 22, 23, 39, 5, 21], simulation [9, 18, 40, 32], and experimental [13, 34, 17, 11, 27] attention due to their thermodynamic and topological stability, their small size, and their inherent property of easy movement and repositioning under the application of low or even tiny in-plane electric currents. They seem promising for use in next generation spintronic devices [33, 50] as information carriers, giving the credentials of ultra dense low-cost power storage and the capability to perform logical operations [12]. The next generation magnetic memory devices would rely on the efficient creation and control of magnetic textures, such as magnetic skyrmions using rather tiny electric currents [35, 29, 7, 19]. The aforementioned topological stability is related to the confined skyrmion magnetic configuration, which is predicted to be stable because the individual atomic spins, oriented opposite to those of the surrounding thin-film cannot perform flipping motion. Spins hindered to align themselves with the rest of atoms in confined geometry without overcoming an energy barrier. The origin of the energy barrier is attributed to the “topological protection”. The thermodynamic stability of skyrmions is considerably strong and can be attributed to the particular magnetic configuration which can be characterized by a total topological charge described by skyrmion number $S$ [23]. This skyrmion number $S$ is an integer and to this point is being considered having quantized values that cannot be changed continuously. The skyrmion

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number $S$ is defined as

$$ S = \frac{1}{4\pi} \int_A q_{Sk} \, dA $$  \hspace{1cm} (1) $$

where $q_{Sk}$ is given by the following relation

$$ q_{Sk} = \mathbf{m} \cdot (\frac{\partial \mathbf{m}}{\partial x} \times \frac{\partial \mathbf{m}}{\partial y}). $$  \hspace{1cm} (2) $$

The quantity $\mathbf{m}$ is the unit vector of the local magnetization defined as $\mathbf{m} = M/M_s$ with $M$ being the magnetization and $M_s$ the saturation magnetization. The skyrmion number $S$ is a physical and topological quantity that measures how many times $\mathbf{m}$ wraps the unit sphere [47]. The integrated quantity describes the topological density $q_{Sk}$ and has units of nm$^{-2}$, which are implied throughout the manuscript. In many instances the integrated quantity is also referred as “topological charge”. Surface $A$ is the surface domain of integration and corresponds to the upper or the lower triangular bounding surface of the FePt nanoelement under investigation.

The magnetization reversal in 330 nm triangular prism magnetic nanoelements with variable magnetocrystalline anisotropy (as that of partially chemically ordered FePt) has been studied using Finite Elements micromagnetic simulations in [38]. The simulation results showed that a wealth of reversal mechanisms is possible sensitively depending on the uniaxial magnetocrystalline anisotropy values and directions; the latter may explain the different Magnetic Force Microscopy patterns obtained in such magnetic systems. In addition, the micromagnetic simulations revealed that interesting vortex-like formations can be produced and stabilized in large field ranges and in sizes that can be tuned by the magnetocrystalline anisotropy (MCA) of the material. The aforementioned spontaneous ground states of skyrmion-like configurations were obtained and in other magnetic systems without the implication of chiral interactions such as Dzyaloshinsky-Moriya (DMI) [45 - 49].

In the present work a quantitative description is given for the vortex-skyrmion configurations by calculating the skyrmion number at 0°C obtained for FePt triangular magnetic nanoislands having variable magnetocrystalline anisotropy. The aforementioned calculation can reveal information not readily recognizable by simple visual-inspection of the micromagnetic configurations. Furthermore, the skyrmion number as a function of the applied field along a hysteresis curve can give quantitative information of the reversal mechanisms and energy barriers involved. In what follows we present examples on the numerical calculation of skyrmion number as means of characterizing magnetic configurations and reversal in nanoelements including thin film asymmetric triangular nanoislands.

2 Micromagnetic modeling

2.1 FEM solution of Landau-Lifshitz-Gilbert (LLG) equation

The rate of change of the dynamical magnetization field $M$ is governed by a nonlinear equation of motion, the Landau-Lifshitz-Gilbert (LLG) equation

$$ \frac{d\mathbf{M}}{dt} = \frac{\gamma}{1 + \alpha^2} (\mathbf{M} \times \mathbf{H}_{eff}) - \frac{\alpha \gamma}{(1 + \alpha^2)|\mathbf{M}|} \mathbf{M} \times (\mathbf{M} \times \mathbf{H}_{eff}). $$  \hspace{1cm} (3) $$

In the aforementioned LLG equation $\alpha > 0$ is a phenomenological dimensionless damping constant that depends on the material and $\gamma$ is the electron gyromagnetic ratio. The effective field that governs the dynamical behavior of the system has contributions from various effects that are of very different nature and can be expressed as $\mathbf{H}_{eff} = \mathbf{H}_{anis} + \mathbf{H}_{exch} + \mathbf{H}_{anis} + \mathbf{H}_{demag}$. Respectively, these field contributions are the external magnetic field $\mathbf{H}_{ext}$, the exchange field $\mathbf{H}_{exch}$, the anisotropy field $\mathbf{H}_{anis}$ and the demagnetizing field $\mathbf{H}_{demag}$.

For the solution of the LLG equation We have performed micromagnetic finite element calculations using the Nmag software [8]. The dimensionless damping constant $\alpha$ was set to 1 in order to achieve fast damping and reach convergence quickly as we are interested in static magnetization configurations. The default convergence criterion for each applied external field step $\mathbf{H}_{ext}$ was that the magnetization should move slower than 1 degree per nanosecond, globally or on average for all spins. The sample was described as a triangular prism with equilateral triangle base of 330 nm and 36 nm in height and is shown in Fig. 1

Fig. 1: Model geometry and the generated mesh.

The 36 nm thickness of the film matches that reported in [25] while Okamoto in [31] suggests 24 nm, which is comparable and not expected to lead to qualitatively different behavior. The following frame of reference axes assignment convention was used: $x$ along the triangle height, $y$ along the side perpendicular to $x$, and $z$ perpendicular to the film plane. The considered finite element mesh for the triangular film under study was generated using the automatic three dimensional (3D) tetrahedral mesh generator Netgen [52]. We have used a 3.4 nm maximum distance between nodes which is lower than the value of the exchange length $l_{ex} = \frac{2A}{\mu_0 M_s^2} \approx 3.5$ nm. This resulted in 488874 vol-
2.2 Skyrmion number computation

The calculation of skyrmion number $S$ necessitates the knowledge of the computed normalized magnetization vector $\mathbf{m}$ obtained from the solution of LLG equations. Once the finite element approximation of the normalized magnetization $\mathbf{m}_h$ has been computed, the skyrmion number $S_h$, following [1], is approximated by

$$S_h = \frac{1}{4\pi} \sum_{e=1}^{N_e} \mathbf{m}_h^e \cdot \left( \frac{\partial \mathbf{m}_h^e}{\partial x} \times \frac{\partial \mathbf{m}_h^e}{\partial y} \right) |A_e|,$$  

where $m_h, S_h$ are the discrete representations of $m, S$ respectively with $e$ denoting the element and $N_e$ the total number of elements used for the surface domain discretization. It should be noted that throughout the manuscript the symbol $S$ instead of $S_h$ will be used for the computed value of the skyrmion number. The integration takes place over the top or bottom surface boundary of the prism $A$. Since we are using tetrahedral P1 elements for the discretization of the prism volume, the top (or bottom) surface boundary is comprised of triangles with outwards pointing normal parallel to the $\hat{z}$ unit vector. Magnetizations are extracted for the top or bottom surface of the magnetic prismatic nanoelement. These particular magnetizations located on the surface elements of the two bases are used for the actual computations of $S$ and of the relative topological quantities. It is possible for a magnetic configuration to include more than one skyrmion. Inevitably, the total skyrmion number would be the algebraic sum of its individual skyrmionic configurations. It follows that a structure that locally includes several skyrmions of different polarity or chirality may yield a zero total skyrmion number. The physical significance of this situation may be attributed to the fact that structures with opposing $S$ may be easier to mutually annihilate. Therefore, it is of interest to monitor following [9] the integral of the absolute value of the topological density symbolized with $S_{abs}$ as it describes the existence of topological entities that are masked and washed out when $S$ is calculated through the integral over all surface domain $A$. The quantity $S_{abs}$ is defined by the relation

$$S_{abs} = \frac{1}{4\pi} \int_A \left| \mathbf{m} \cdot \left( \frac{\partial \mathbf{m}}{\partial x} \times \frac{\partial \mathbf{m}}{\partial y} \right) \right| dA$$  

(5)

The scalar quantity $S_{abs}$ is injective and provides the necessary distinctness for different skyrmionic states [9]. The stabilization of such magnetic skyrmions is usually linked to the existence of some kind of anisotropic Dzyaloshinskii-Moriya interaction (DMI). Its discrete estimation follows similarly to [3]. It is interesting the calculation of skyrmion numbers for micromagnetic configurations in nanoelements since it can reveal information not readily recognizable by simple visual inspection of the micromagnetic configurations. Furthermore, the skyrmion number $S$ as a function of the applied field $H_{ext}$ along an hysteresis curve can provide quantitative information of the reversal mechanisms and energy barriers involved in the process.

3 Results

3.1 In-plane MCA

In the first system studied the magnetocrystalline anisotropy (MCA) lies within the plane of the triangular nanoelement parallel to $x$-direction ($\mathbf{K}/[100]$) with the external field $H_{ext}$ applied along the width of the nanoelement which is parallel to $z$-direction ($H_{ext}/[001]$). The $H_{ext}$ direction is being fixed parallel to $z$-direction throughout this work for all systems studied. We have calculated the half-hysteresis loop (descending branch of the loop) for the triangular prismatic nanoelements for different MCA values. The $K_u=100kJ/m^3$ is presented in Fig. 2 along with $q_{sk}$. Some micromagnetic configurations being formed along the path of the reversal are shown in Fig. 3. We present results only for a declining external field $H_{ext}$ since the full hysteresis diagram does not contribute any additional information regarding the magnetization reversal process [35]. Presenting the full hysteresis diagram would inevitably doubled the required computational effort.
Magnetization reversal depicted in Fig. 2 starts when the normalized magnetization decreases from the saturation value $M/M_s = 1$, and passing through the nucleation field it reaches $M/M_s = 0$. Then after passing the annihilation field, it attains finally the value $M/M_s = -1$ indicative that all spins have reversed their magnetization vector orientation. During this reversal process the values of $S$ and $S_{abs}$ are computed in order to provide a quantitative description of the skyrmion-like localized configurations in conjunction with the qualitative actual visualization of the normalized magnetization vector $\mathbf{m}$ of the individual spins. Values of $S$ have been calculated for the top and bottom surface of the triangular prismatic nanoelement for various $Ku$ values shown in Fig. 4 for all magnetic systems in the present investigation. The values of $S$ have the same quantitative and qualitative behavior on top and bottom surface of the nanoelement ensuring the consistency of the numerical calculations. Throughout the manuscript the reported values of skyrmion numbers $S, S_{abs}$ refer to the computed values on the top surface of the nanoelement.

For the MCA value $Ku=100\text{kJ/m}^3$ represented in Fig. 2 the process of the reversal of spins gives birth to vortex like formations. The value of $S$ emerges from zero and gradually increases; attaining value $0.5$, characteristic of magnetic vortex for external magnetic field $H_{ext}=4.0 \times 10^5 \text{A/m}$, it reaches the maximum value of $S \approx 0.75$ that can be considered as an incomplete skyrmion for field value close to $H_{ext} = -2.1 \times 10^5 \text{A/m}$. Note that similar non-integer values of skyrmion number have been reported in confined helimagnetic nanostructures and in thin confined polygonal nanostructures. It is anticipated that in the present finite magnetic system the skyrmion number can be non-integer due to the restricted area of integration $A$ in Eq. 1 and Eq. 5 and the essential contribution of magnetostatic energy. The value of $S = 0.5$ describes a vortex like micromagnetic configuration.

Around the external field value of $H_{ext} = 9.2 \times 10^5 \text{A/m}$ a small step can be detected in the variation of $M/M_s$ reflected also in $S$ and magnified in the injective property $S_{abs}$ indicating the origin of magnetization reversal through vortex or skyrmion type mechanisms. In addition, around $H_{ext} = 2.6 \times 10^5 \text{A/m}$ a jump discontinuity is evident both for $S, S_{abs}$ not captured by the magnetization curve $M/M_s$. A second jump discontinuity on $S$ is evident around $H_{ext} = -2.7 \times 10^5 \text{A/m}$ causing the change of $S$ value approximately from 0.7 to -0.4 (relative variation 157%). The aforementioned variation is followed by a change of the sign of $S$ characteristic for a change in the polarity of the vortex type micromagnetic configuration. Further decrease
of the external magnetic field causes the continuous decay of $S$ and its annihilation after the final stage of the reversal process. The magnification of jump discontinuities in $S_{abs}$ is anticipated since it is injective and provides the necessary distinctness for different skyrmionic and consequently energy states. Therefore, it is being used in order to detect and explore possible energy barriers during the reversal process. Additionally, in Fig. 2 differentiation of shapes describing $S, S_{abs}$ reveals that there are local topological density $q_{sk}$ regions-domains which sum up to zero and therefore mutually annihilate.

Visualizations of micromagnetic configurations are shown in Fig. 5 for the representative selected external field values depicted in Fig. 2 and designated as A, B, C, D. The actual topological density $q_{sk}$ defined in Eq. 2 represents the ‘local’ skyrmion number of the surface element and is also visualized in Fig. 5. This enriched representation gives both qualitative and quantitative description of the actual magnetization configuration. The existence of domains with augmented local topological density is observed close to upper and lower corners of the nanoelement along $y$-direction for A, B and D points. In addition, an elliptical domain can be observed along the $x$-axis which is also the direction of the in plane MCA $K_u=100\text{kJ/m}^3$, at the center of the triangular base present in all characteristic points A, B, C, D. These three magnetic entities can be considered as incomplete skyrmions and are present for a wide range of external field values. In Fig. 3 (point A) the aforementioned magnetic entities expose different magnetization circulations. Those in the corners have a counter clockwise circulation while the domain with augmented $q_{sk}$ at the center of the triangle has a clockwise circulation.

In Fig. 5 skyrmion number $S$ as a function of the external field $H_{ext}$ for different values of $K_u$ is shown. As the magnitude of MCA increases gradually starting from $K_u=100\text{kJ/m}^3$ a similar behavior with Fig. 2 is observed regarding the qualitative and quantitative characteristics of $S$. In the cases of $K_u = 150, 250, 350\text{kJ/m}^3$ the skyrmion number attains lower values as $K_u$ increases exhibiting jump discontinuities. The calculated maximum (or negative minimum) values denoted as $S_{max}$ for the aforementioned cases do not exceed the value $S_{max}=0.7$ for $K_u=100\text{kJ/m}^3$ represented in Fig. 5. For $K_u=200$ and $300\text{kJ/m}^3$ $S$ attains maximum values 0.55–0.50 respectively but at different external magnetic field values $H_{ext}$. It is evident that the magnetization reversal mechanism necessitates the formation of incomplete skyrmions ($0.5 < S < 1$), vortex-like states ($S = 0.5$) not only for low $K_u=100$ and $150\text{kJ/m}^3$ values but also for the considered as intermediate values of $K_u=250, 350\text{kJ/m}^3$ (Fig. 6). Further increase of MCA’s values to $K_u = 400, 450, 500\text{kJ/m}^3$ expose similar reversal characteristics with $S_{max}$ establishing a plateau region at 0.5 shown in Fig. 6 characteristic for vortex like reversal process.

The discontinuities detected in case of $K_u=100\text{kJ/m}^3$ are present not only for different values of $K_u$ but for different orientation of the MCA with respect to the surface of the nanoelement e.g. parallel to $z$-direction. They need further clarification and can be associated to the rich energetic environment having contributions from demagnetization $E_{\text{demag}}$, exchange $E_{\text{exchange}}$ and anisotropic $E_{\text{anis}}$ energies which can be computed for the systems studied in the present work. Complicated and rich energetic landscapes on the surface of the nanoelement are anticipated. The skyrmion formation is related to the interplay of these energetic contributions.

In order to measure the effect of each individual energy type on the micromagnetic configuration during the magnetization reversal process the absolute relative energy difference $\Delta E_{\text{rel}}^{\text{type}} = \frac{|E_{\text{tot}}^{\text{type}} - E_{\text{tot}}^{\text{max}}|}{E_{\text{tot}}^{\text{type}}} \times 100(\%)$ (where type stands for anis, exch, demag) is computed between the consecutive external magnetic field values $H_{ext}, H_{ext+1}$. As mentioned in Section 2 the external magnetic field step between consecutive field values is $\delta H_{ext}=4\text{kA/m}$. The values of the relative differences of anisotropy, demagnetization and exchange energies are shown in Fig. 7 as functions of $H_{ext}$ for MCA values of $K_u=100, 150\text{kJ/m}^3$ superimposed with $S_{abs}$. It is clear that even in the first steps of the magnetization reversal around values 8.5–9.5 $\times 10^5\Lambda/m$ of the external field for $K_u=100\text{kJ/m}^3$ small steps of the skyrmion number are induced by jump discontinuities on the relative energies and vice versa. These jump
discontinuities represent the actual energy barriers are pronounced for all types of energies at the beginning of the reversal process with $E_{\text{anis}}$ being the more prominent compared to $E_{\text{demag}}, E_{\text{exch}}$. The magnetic system and its associated energy should overcome a significant energy barrier in order to start the reversal process in the confined triangular prismatic nanomagnet. In particular, $\Delta E_{\text{anis}}$ attains values close to 42%. Further reduction of the external magnetic field shows continuous behavior up to the value of $H_{\text{ext}} = 2.5 \times 10^5 \text{A/m}$ for $S_{\text{abs}}$. The decrease of the external field $H_{\text{ext}}$ drives the continuous and gradual formation of an incomplete skyrmion ($S < 1$). This continuous behaviour is dictated from the continuous behaviour of the total magnetization energy and its energetic components $E_{\text{anis}}, E_{\text{demag}}, E_{\text{exch}}$. A new energy barrier is observed for $S_{\text{abs}}$ around $H_{\text{ext}} < 2.5 \times 10^5 \text{A/m}$ for the exchange energy $E_{\text{exch}}$ not followed by the other calculated energies. The value $\Delta E_{\text{exch}}$ of this discontinuity is close to 10%. It is clear that this sharp change at $E_{\text{exch}}$ induces the incomplete skyrmion discontinuity not only for $H_{\text{ext}} < 2.5 \times 10^5 \text{A/m}$ but also for the symmetric with respect $H_{\text{ext}} = 0 \text{A/m}$ second maximum around $H_{\text{ext}} = 2.5 \times 10^5 \text{A/m}$.

In particular, for external fields in the vicinity of $H_{\text{ext}} = 0 \text{A/m}$ a steep descent is evident for $\Delta E_{\text{demag}}$. Energy component $\Delta E_{\text{anis}}$ shows a smoother behavior between the first and last discontinuities having a declining behavior in the first half of the magnetization reversal process where the external field approaches zero value. A continuous increase of the relative change $\Delta E_{\text{anis}}$ is profound in the second half and final stage of the reversal process. Relative energy difference $\Delta E_{\text{exch}}$ exhibits an interesting non-continuous behavior having a significant number of sharp discontinuities in the range of $H_{\text{ext}} = (-2.5 \text{ to } +2.5) \times 10^5 \text{A/m}$ external field values. Calculation of energies and relative energies differences for varied $K_u$ showed similar qualitative and quantitative characteristics with the case of $K_u = 100 \text{kJ/m}^3$. Vortex like or incomplete skyrmion states are triggered by abrupt energy changes and energy barrier crossings.

Further calculations have performed by changing the direction of MCA from $x$ to $y$ direction. This directional change of MCA gives similar physical results regarding the formation of vortices despite the fact that MCA’s direction remains in plane. This situation with MCA along y-direction differs from MCA lying along x-direction only with respect to the subtle effects of the edge curling on the nucleation process.

### 3.2 Perpendicular MCA

It is challenging to investigate the effects associated with MCA when is set to $z$-direction which is the direction normal to the basis surface of the triangular FePt nanoelement. As the vortex-like formations in this system arise from the competition of exchange and magnetostatic energies it is expected that these phenomena will be more pronounced when there is a perpendicular MCA which leads to strong demagnetizing fields. The numerical calculations showed that the dependence of $S$ for the lowest MCA value $K_u = 100 \text{kJ/m}^3$ is quite similar to the case of in-plane MCA directions exhibiting the same magnetization reversal process. The magnetic system case with $K_u = 150 \text{kJ/m}^3$ is presented in Fig. 8. Since the $K_u$ value is not high enough to give perpendicular anisotropy as the $H_{\text{ext}}$ is reduced the system departs from saturation through a series of topologically non-trivial formations giving a gradual increase of the skyrmion number which attains the maximum value $S = 42\%$ in a plateau region between $H_{\text{ext}} = -2.5 \times 10^5 \text{A/m}$ and $H_{\text{ext}} = -5 \times 10^5 \text{A/m}$ is evident. The aforementioned gradual increase of the skyrmion number $S$ for MCA parallel to $z$-direction for all $K_u$ values studied starts at lower external field values compared to systems having in plane MCA direction. This external field values retardation can be attributed to the higher energy barrier needed to overcome in order to start the reversal process through skyrmion formation. The critical field signaling skyrmion formation for the different $K_u = 150, 250, 350\text{kJ/m}^3$ values for MCA parallel to $z$-direction is located around $H_{\text{ext}} = 3.5 \times 10^5 \text{A/m}$ (Fig. 8) and is considerably lower compared to the external field value of $H_{\text{ext}} = 7.5 \times 10^5 \text{A/m}$ for in-plane MCA (Fig. 2).

The behavior is strikingly different when MCA attains the values of $K_u = 250, 350\text{kJ/m}^3$ depicted also in Fig. 8. For the case where $K_u = 350\text{kJ/m}^3$ skyrmionic configurations having negative values emerge for external field values lower than $5.0 \times 10^5 \text{A/m}$. The micromagnetic configuration in Fig. 5 hosts one skyrmion located at the center of the nanoparticle. A counter-clockwise circulation (positive circulation) can be identified on the top view of the nanoparticle. The central spins of the skyrmion point inwards (negative polarity) as clearly presented at the bottom view of the spin configuration. Consequently, chirality which is the product of circulation and polarity is negative dictating in this manner the negativity of the skyrmion number.

For the particular case of $K_u = 250\text{kJ/m}^3$ regions hosting skyrmions are evident having skyrmion number values close to $S = 3$ in a range of applied external fields from $H_{\text{ext}} = -0.3 \times 10^5 \text{A/m}$ to $-5.3 \times 10^5 \text{A/m}$. In Fig. 9 micromagnetic configurations with topolog-
When skyrmion number attains negative values with respect to top view by 60 degrees) for configuration in top and bottom view (rotated parallel to z-direction alongside with the micromagnetic fields $K_u$.)

Maximum of skyrmion number $S$ discontinuity with actual value close to $S = 1$. The respective isosurfaces of $q_{sk}$ for point B reveal the existence of one skyrmion located at the center of the triangular prismatic nanoelement.

Points C, D represent micromagnetic configurations hosting three skyrmions. The centers of the skyrmions define an equilateral triangle in both micromagnetic configurations. The essential difference of the skyrmions present in C and D points is their actual size. Skyrmions of point C are larger compared to the respective three skyrmions in D although they have the same circular shapes and location. This can be attributed to the fact that while the sizes in skyrmions of C (Fig. 9 (C)) are larger than those of D (Fig. 9 (D)) the topological densities $q_{sk}$ are higher in D in order to compensate the lower skyrmion surface contributing to the total triangular surface base integration giving in both cases C and D a total skyrmion number equal to 3. Representative values of the maximum $q_{sk}$ on the surface element are $q_{sk,C} = 0.003462 < q_{sk,D} = 0.02181$.

In Fig. 6 the maximum values of $S$ denoted as $S_{max}$ are reported for MCA parallel to z-direction. Moreover, representative configurations depicted for external field values corresponding to $S_{max}$ showing $q_{sk}$ superimposed with magnetization are presented in Fig. 10. For the case where $K_u = 200kJ/m^3$ at the center of the triangular base a clear and complete skyrmion emerges. It has an almost perfect circular shape with the higher values of $q_{sk}$ located at the center mitigating when moving away but along the circle’s radius. The magnetization vectors have a counter-clockwise circulation around the skyrmion. In case where $K_u = 250kJ/m^3$ and $S_{max} ≈ 3.25$ extended regions located at the triangle’s vertices running along the edges of the triangular base are evident. This magnetic configuration significantly differs from the configuration having three well developed skyrmions defining segregated and distinct regions presented in Fig. 9 (point C). These multiple skyrmions or clusters of skyrmions on the surface of the triangular disk are evident and the actual calculation of $S$ gives values during the reversal process in the range of $1 ≤ S < 4$ for all MCA values studied having perpendicular anisotropy. The maximum value $S_{max} = 3$ for the case of $K_u = 300kJ/m^3$ is also depicted in Fig. 10 exposing three skyrmions located in extended circular regions.

The increase of the MCA value from $K_u = 150kJ/m^3$ to $500kJ/m^3$ plays a dramatic effect in the magnetization reversal process and the creation of skyrmion regions. Particularly, in the cases where $K_u$ attains values beyond $300kJ/m^3$ reaching $500kJ/m^3$ the maximum of skyrmion number $S$ establishes a plateau at $S = 2$ indicative of the formation of two skyrmions on the surface of the nanoelement. The case of $K_u = 350kJ/m^3$ where $S_{max} = 2$ is representative and is shown in Fig. 10. The two skyrmions are exactly located along the height of the triangle (parallel to x-direction) having different shapes resembling different perturbations of the circular shape. The formation and actual detection of skyrmions can be revealed by visual.
alizing the actual reversal process. A quantitative and coherent picture can be provided by the calculation of $S$.

Computations of relative energy differences accompanied by $S_{abs}$ are depicted in Fig. [11] for $K_u = 250 \text{kJ/m}^3$ which is the case showed the formation of three skyrmions. As it is already commented the first steps of the magnetization reversal for MCA normal to nanoelement’s surface start at external field values $H_{ext}$ significantly lower ($< 5 \times 10^5 \text{A/m}$) compared to the case of in-plane MCA. Following $S_{abs}$ and relative energies variation with respect to external field, energy barriers are present around $H_{ext} = 5 \times 10^5 \text{A/m}$ for all the components of energy. Particularly in Fig. [11] for $K_u = 250 \text{kJ/m}^3$, $\Delta E_{\text{rel}}^{\text{exch}}$ is close 90% and is the most prominent jump discontinuity compared to $\Delta E_{\text{ani}}$, $\Delta E_{\text{demag}}$ whose jumps are around 10%. It should also noted that $E_{\text{ani}}$ exhibits a 90% jump, which is twice as much as the one observed in the case of in plane anisotropy at $K_u = 100 \text{kJ/m}^3$ which was calculated to 42%. The reduction of the external magnetic field affects in a continuous manner the different magnetic energies up to the value of $H_{ext} = 0 \text{A/m}$. In the vicinity of the zero for negative external fields new jump discontinuities are evident for all energies. The decrease of external field $H_{ext}$ drives the continuous and gradual formation followed by energetic and therefore skyrmionic discontinuity events. Complete and incomplete skyrmions are present having values $1 < S < 4$. Rich energy patterns and textures are clear having similar behaviour not only for $K_u = 250 \text{kJ/m}^3$ but for all $K_u$ values studied when MCA is normal to the nanoelements’ base.

**Fig. 12** represents the relative energies for characteristic points selected from Fig. [11] at $K_u = 250 \text{kJ/m}^3$. Energies $E_{\text{ani}}, E_{\text{exch}}, E_{\text{demag}}$ are grouped and shown in five different points. The grouped energies $\{A_i, D_i, E_i\}$ associated with point $i$ ($i = 1, ..., 5$) are depicted at the same or approximately the same $H_{ext,i}$ value. At point A1 before crossing the energy barrier, $E_{\text{ani}}$ develops an inner triangular region with values lower compared to the maximum values located at the sides of the nanoelement’s base. At A2 point where the barrier is being crossed and skyrmion has been formed the energy distribution follows the skyrmion’s location with increasing values of $E_{\text{ani}}$ radically moving from the center towards the outer circular domain of skyrmion. Energy isosurfaces for point A3 expose three new developed regions in the vicinity of the nanoelement’s base vertices. Point A4 represents a local energy minimum of $E_{\text{ani}}$, from around the skysmion domain at the center well developed stripe-like energy domains running parallel to nanoelement’s edges are evident. Point A5 is the location where the highest energy barrier is detected. From the contour plot is evident that the energy follows exactly the location of the multiple skyrmions formed. Calculation of $E_{\text{demag}}$ provides the same qualitative behaviour with the subtle difference on point D1 at almost identical $H_{ext}$ value with A1 where $E_{\text{demag}}$ has a uniform distribution on the nanoelement’s base. The calculated exchange energy $E_{\text{exch}}$ distribution follows the formation process of skyrmions. At point E1 high energy regions are located at the vertices of the nanoelement in contrast to $E_{\text{ani}}$. The competition between these energies and energy barrier crossings gives birth to skyrmion magnetic configurations.

### 3.3 MCA parallel to [111]

In addition to MCA lying on the surface or being normal to the surface of the nanoelement the magneto-crystalline anisotropy is set parallel to [111] direction. The latter case is of interest as in many instances

![Image of micromagnetic configurations](image-url)
3.3 MCA parallel to [111]

Results

Figure 12: Demagnetization, exchange, and anisotropic energies for $K_u = 250 \text{kJ/m}^3$ for selected points during the reversal process chosen from Fig. 11.

FePt and CoPt films tend to grow with their [111] crystallographic directions resulting an angle of 54.7° to the film normal [1]. The numerical simulation results are presented for $S$ in Fig. 4 as a function of $K_u$ fixing external field value at $H_{ext}=0 \text{A/m}$. At $K_u = 100 \text{kJ/m}^3$ skyrmion number is close to value $S = 0.7$. By increasing MCA up to $K_u = 250 \text{kJ/m}^3$ skyrmion number reduces attaining negative but non-zero values for external field $H_{ext}=0 \text{A/m}$. This is an interesting fact and significantly differentiates compared to the cases where MCA is in-plane or perpendicular to the nanoelement’s base. For $S_{max} < 0$ the respective MCA value range is $K_u = 150−350 \text{kJ/m}^3$. Calculation of the skyrmion number at different external field values for the representative $K_u = 150, 250, 350 \text{kJ/m}^3$ values are shown in Fig. 13. Evident is the manifestation of micromagnetic configurations mainly having negative skyrmion numbers for external fields ranging from $H_{ext}=5 \times 10^5 \text{A/m}$ to approximately $H_{ext} = -2 \times 10^5 \text{A/m}$. The minimum value of $S$ is observed for the case of $K_u = 150 \text{kJ/m}^3$ and is close to $S = -0.4$. For the three different $K_u$ values shown
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Table 1: $S$ as a function of $H_{ext}$ for $Ku = 150, 250, 350 \text{kJ/m}^3$ with MCA running parallel to [111] direction alongside with the micromagnetic configuration in top and bottom view (rotated with respect to top view by 60 degrees) for representative point P with $S < 0$ at $Ku = 350 \text{kJ/m}^3$.

Figure 13: the crossover to negative $S$ happens at $H_{ext} = 5 \times 10^5 \text{A/m}$. Also the maximum antivortex states are located at the vicinity of zero external magnetic field which significantly differentiate compared to the previous studied cases.

Conclusions

The topological invariant known as skyrmion number $S$ has been calculated for FePt triangular prism nanonelements with different directions and magnitude of MCA for varying magnitude of the external magnetic field $H_{ext}$. The direction of the external field $H_{ext}$ was normal to nanoelement’s surface in all conducted numerical simulations. Magnetization configurations during reversal process were studied. It was possible to explore the formation of skyrmionic regions and qualitatively-quantitatively characterize them by a variety of calculated properties such as the skyrmion number, the different contributions on the magnetic energy such as demagnetization energy, exchange energy and uniaxial anisotropy energy and visualization of the micromagnetic configurations. Skyrmionic magnetic configurations have been detected in high symmetry positions with respect to the geometry of the triangular prism having skyrmion number greater than one ($S > 1$) for the case where MCA was normal to nanoelement’s base. For MCA attaining values between $Ku = 200 - 500 \text{kJ/m}^3$ three distinct skyrmions are formed and persist for a range of external fields.

In conjunction with previous studies it is clear that magnetic skyrmions can be produced in a wide range of external fields just by tuning MCA’s magnitude and direction, even in the absence of chiral interactions such as Dzyaloshinsky-Moriya. It is challenging to extent the numerical simulations including thermal effects in the form of Brownian term in LLG equation in order to investigate the formation of skyrmions at room temperature.

Acknowledgments

V.D. Stavrou would like to thank the State Scholarship Foundation of Greece (IKY) for the financial support under the scholarship grant (appl. no.14386). We would like to thank Mr. Costas Dimakopoulos for his technical support. Computations have been performed at the Laboratory of Mathematical Modeling and Scientific Computing of the Materials Science Department of the University of Ioannina.

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