*Citation for published version:*
Knittel, A, Franchin, M, Nasirpouri, F, Bending, SJ & Fangohr, H 2012, 'Effect of rounded corners on the magnetic properties of pyramidal-shaped shell structures', Journal of Applied Physics, vol. 111, no. 7, pp. 07D127. https://doi.org/10.1063/1.3679073

*DOI:*
10.1063/1.3679073

*Publication date:*
2012

*Document Version*
Publisher's PDF, also known as Version of record

Link to publication

# Effect of rounded corners on the magnetic properties of pyramidal-shaped shell structures

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(Presented 3 November 2011; received 23 September 2011; accepted 1 December 2011; published online 12 March 2012)

In recent years, the advance of novel chemical growth techniques has led to the fabrication of complex, three-dimensional magnetic nanostructures. The corners and edges of such realistic geometries are generally not sharp but rounded. In a previous article we have argued that high demagnetization fields in the vicinity of sharp edges lead to the formation of an asymmetric vortex state in pyramidal-shaped magnetic shell structures. The asymmetric vortex state is potentially interesting with respect to future magnetic memory devices. In this work a micromagnetic model is used to investigate the effect of rounded corners and edges on the magnetic reversal process within these pyramidal-shaped magnetic shell structures. In particular, we explore the degree of rounding, which has to be introduced in order to suppress the asymmetric vortex state. Another emphasis is placed on the magnetic reversal of (quasi-)homogeneous states within these structures. We demonstrate that the rounding of corners significantly reduces the coercivity. This complies with former studies on cuboidal structures, which suggest the important effect of corners on the magnetic reversal of homogeneous magnetic states. The present study uses a finite-element discretization for the numerical solution of the micromagnetic equations, which provides flexibility with respect to the modeling of complex shapes. In particular, this method is very accurate with respect to structures with a smooth surface. © *2012 American Institute of Physics*. [doi:10.1063/1.3679073]

## I. INTRODUCTION

In micromagnetic studies one usually investigates idealized geometries such as rectangular prisms, which approximate realistic structures grown in experiments. This is also a result of the fact that most micromagnetic studies are based on a finite difference discretization, which is only accurate in the case of cuboidal structures.[1] However, realistic structures contain non-ideal features like surface roughness and a rounding of corners and edges. The important effect of a rounding of corners and edges on the formation of magnetic states has already been demonstrated before.[2,3]

In a recent article we have studied the magnetic properties of pyramidal-shaped nickel shells.[4,5] In this article we introduce a rounding of corners and edges to these structures and consider two scenarios:

(1) The magnetic reversal of a quasi-homogeneous state along the easy-axis direction.
(2) A magnetic reversal at larger structure sizes, at which the asymmetric vortex state forms at remanence in the absence of rounding.

In the former case the corresponding reversal curve has a square-like shape and a high remanent magnetization in the absence of rounding.[4] The introduction of a rounding should lead to a reduction of the coercivity field, as, analogous to the macro-spin model of ellipsoidal geometries, the reversal process becomes more homogeneous. The expected higher degree of homogeneity of the remanent state should not have a strong effect on the spatially averaged magnetization. Consequently, only minor modifications in the remanent magnetization are expected. These *a priori* assumptions are confirmed by the investigations in this article.

The asymmetric vortex state is observed for scenario (2) in the absence of any rounding. As the formation of this state is due to the occurrence of high local demagnetization fields in the vicinity of sharp edges (Section 4.1.4 in Ref. 4), it should be suppressed in the presence of a sufficient degree of rounding. This article investigates which degree of rounding leads to such a suppression.

## II. METHODOLOGY

We use the same approach as in Ref. 4, i.e., we use a simple micromagnetic model, in which we do not consider the magnetocrystalline anisotropy. For our fundamental study it is advantageous to use such a simple model, so that effects from the rounding of corners become as prominent as possible. The saturation magnetization is set to $M_S = 493\,380\ \mathrm{A\ m^{-1}}$ and the exchange constant to $A = 7.2 \times 10^{-12}\ \mathrm{A\ m^{-1}}$.[6] The finite-element based solver NMAG is used to solve the micromagnetic equation numerically.[7] The geometrical model is based on the pyramidal-shaped geometry presented in Ref. 4. Thus, the size of the structure is determined by the edge length $a$ of the square base, while the height of the structure is kept fixed at

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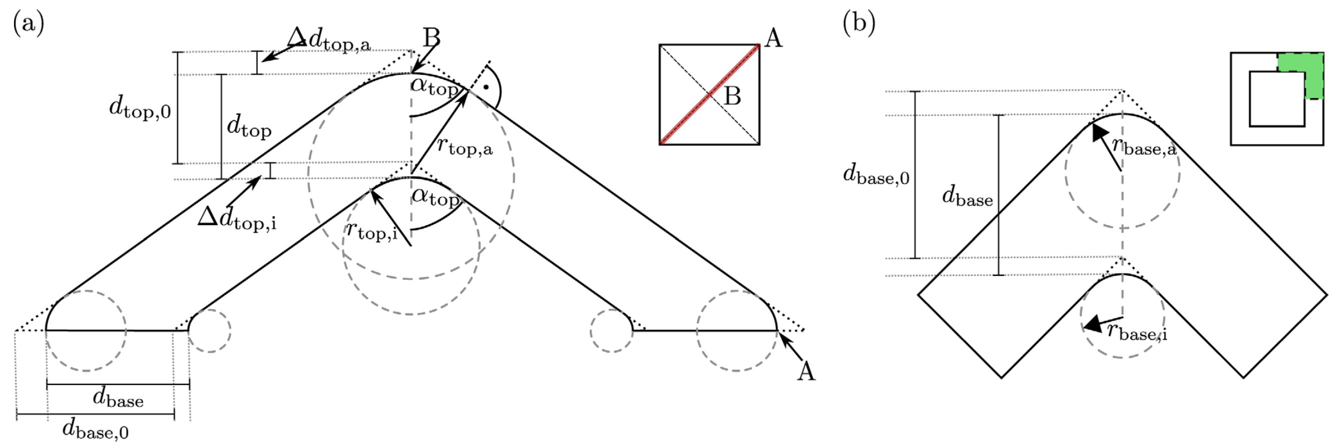


FIG. 1. (Color online) (a) The small inset on the top right shows the pyramidal shell from a top-down perspective. The marked diagonal refers to the cross-section shown in the figure. The geometry without a rounding is given by the dotted lines (visible at the corners). The rounding is introduced by replacing these corners by part-circles, the corresponding full circles are visualized by the dashed lines. Thus, the rounding at the tip is defined by the corresponding radii $r_{top,i}$ and $r_{top,a}$. However, in this article the variables $d_{top}$ and $r_{top,a}$ are used. (b) The inset on the top right shows the base of the pyramidal shell with the highlighted corner corresponding to the section shown in Fig. 1(b). As for the tip we define the rounding at the corners of the base by using the equivalent parameters $d_{base}$ and $r_{base,a}$. To create a pyramidal shell with rounded corners we then take the following steps: we rigidly sweep the base of the structure along the indicated red path (top right of (a)) between point A at the corner of the base and point B at the tip in order to create a three dimensional (3D) solid. This is done for all four equivalent corner points of the base so that four corresponding solids are created. By forming the union of these solids a pyramidal shell with rounded edges and corners is created.

$h = a/2$. The shape of the structure is controlled by the thickness $t_{rel}$ of the shell. $t_{rel} = 0.0$ corresponds to an infinitesimal thin shell and $t_{rel} = 100.0$ to a conventional pyramid. Figure 1 shows how a pyramidal shell with rounded corners and edges is created. The rounding leads to four additional parameters ($d_{top}$, $r_{top}$, $d_{base}$, and $r_{base}$), which are also defined in Fig. 1. In the following these additional parameters are presented in a dimensionless form, namely $d^{rel}_{top} = d_{top}/d_{top,0}$, $r^{rel}_{top} = 2/\sqrt{3}r_{top,a}/a$, $d^{rel}_{base} = d_{base}/d_{base,0}$, and $r^{rel}_{base} = 2r_{base,a}/a$, so that they are invariant with respect to a change of the system size. In the following we consistently set $d^{rel}_{base} = d^{rel}_{top} = 1.0$. For the discretization of the micromagnetic equation an unstructured, tetrahedral mesh is used. Criteria for a sufficient mesh resolution are presented in Ref. 4.

Magnetic reversal simulations are performed, in which the external magnetic field is subsequently varied. The direction of the external field is parallel to one of the four equivalent edges of the base of the structure. We define this as the $x$-direction. After each variation of the external field the magnetization is relaxed to a stable configuration. Choosing a sufficiently small step size for the variation of the external field, this approach allows for analyzing the corresponding experimental hysteresis measurements. In the presented simulations the external field is subsequently varied between 3 and $-3$ T. In the regime of low magnetic fields ($|H_{ext}| < 0.05$ T), in which the actual switching of the magnetization occurs, a step size of $\Delta H_{ext} = 0.001\,\mathrm{T} = 10\,\mathrm{G} \approx 800\ \mathrm{A\,m^{-1}}$ is chosen for the reversal of the quasi-homogeneous states. For the reversal of the vortex-like configurations a larger step size of $\Delta H_{ext} = 0.01\,\mathrm{T} = 100\,\mathrm{G} \approx 8000\ \mathrm{A\,m^{-1}}$ has been used at magnetic fields below $|H_{ext}| < 0.05$ T.

## III. NUMERICAL RESULTS

In this section two magnetic reversal scenarios are discussed with regard to the influence of the rounding introduced in Fig. 1.

In Fig. 2 the magnetic reversal is shown for pyramidal-shaped, thin shells ($t_{rel} = 10\%$) with a base edge length of $a = 100$ nm and either no or different degrees of rounding at corners and edges. The graph shows that the coercivity decreases substantially with an increasing degree of rounding. This alone may not be surprising given the pinning effect sharp corners have during a magnetic reversal.[8] However, already a rounding with $r^{rel}_{top} = r^{rel}_{base} = 7.5\%$, i.e., with

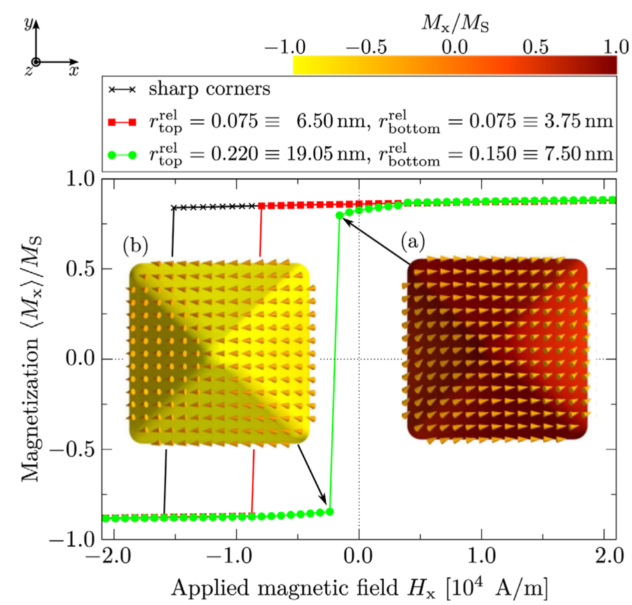


FIG. 2. (Color online) The magnetic reversal along the $x$-direction is shown for pyramidal shells with $a = 100$ nm and $t_{rel} = 10\%$ and different degrees of rounding at the corners and edges. The black curve (crosses) corresponds to the reversal of a pyramidal shell with sharp corners and edges. The geometries corresponding to the green (circles) and red curve (squares) have been created with $d^{rel}_{base} = 1.0$ and $d^{rel}_{top} = 1.0$ and the indicated values for the parameters $r^{rel}_{base}$ and $r^{rel}_{top}$. The two insets show micromagnetic configurations corresponding to the indicated data points of the green curve (circles) (color bar and coordinate axes are shown at the top).

curvature radii below the exchange length of nickel ($l_{\text{exch}} = 6.86\,\text{nm}$), leads to a reduction in the coercivity from $15\,200\,\text{A m}^{-1} < |\vec{H}_{\text{Coerc}}| < 16\,000\,\text{A m}^{-1}$ (black curve with crosses) to $8000\,\text{A m}^{-1} < |\vec{H}_{\text{Coerc}}| < 8800\,\text{A m}^{-1}$ (red curve with squares). The reason is that diverging demagnetization fields, which occur in the vicinity of sharp corners (see Ref. 9 and chapter 3 in Ref. 10), are suppressed even in the presence of just a small degree of rounding. Figure 2 also shows that rounding has not only an important effect on the coercivity but also influences the symmetry of the remanent state. Inset (a) shows an S state (for an accurate definition of this state see Ref. 4) instead of the flower state, which is the remanent state without a rounding.[4] After the reversal a flower state is observed (inset (b) in Fig. 2).

Figure 3 shows the reversal along the $x$-direction within a pyramidal shell with $a = 250\,\text{nm}$ and $t_{\text{rel}} = 50\%$ and different degrees of rounding. In Ref. 4 it has been shown that the asymmetric vortex state plays an important role during this reversal process. Inset (a) of Fig. 3 illustrates the asymmetric vortex state. The core of the vortex state is shifted from the top to the lower side face of the pyramidal-shaped shell. It should be noted that this shift is more pronounced for thinner shell thicknesses (e.g., $t_{\text{rel}} = 10\%$, see Ref. 4). In the illustrated case the shift of the vortex core to the lower side face leads to a net magnetization in the positive $x$-direction. This in-plane net magnetization allows for a switching of the vortex core to the four equivalent side faces, so that, theoretically, an asymmetric vortex state is a realization of a quadbit.[5] During the depicted reversal process the vortex core of the asymmetric vortex moves from the lower side face at

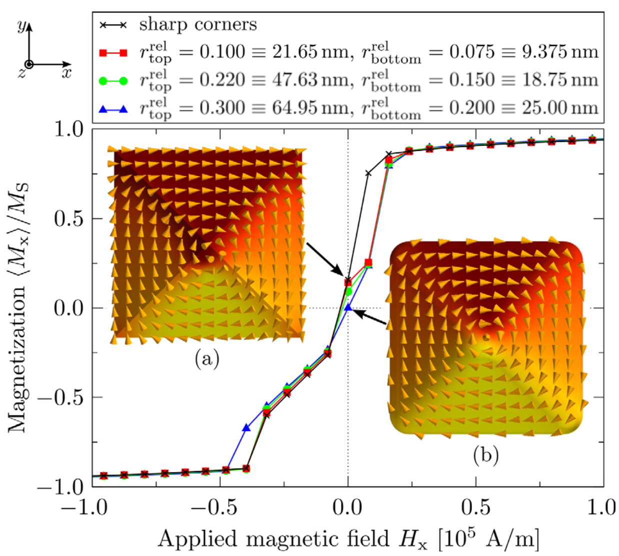


FIG. 3. (Color online) The magnetic reversal along the $x$-direction is shown for pyramidal shells with $a = 250\,\text{nm}$ and $t_{\text{rel}} = 50\%$ and different degrees of rounding at the corners and edges. The black curve (crosses) corresponds to the reversal of a pyramidal shell with sharp corners and edges. The geometries corresponding to the green (circles), red (squres) and blue (triangles) curve have been created with $d^{\text{rel}}_{\text{base}} = 1.0$ and $d^{\text{rel}}_{\text{top}} = 1.0$ and the indicated values for the parameters $r^{\text{rel}}_{\text{base}}$ and $r^{\text{rel}}_{\text{top}}$. The remanent state of the black (crosses), red (squares), and green (circles) data curve (inset (a)) is an asymmetric vortex state, while the remanent state of the blue data curve (triangles, corresponding to the highest degree of rounding) is a symmetric vortex state (inset (b)). The color scheme of the insets corresponds to the color bar in Fig. 2.

remanence to the upper side face at $H_{\text{ext}} = -8000\,\text{A m}^{-1}$ (for the black (crosses), red (squares), and green (circles) data curves in Fig. 3). Figure 3 also shows that a rounding of about $r^{\text{rel}}_{\text{top}} = 30\%$ and $r^{\text{rel}}_{\text{base}} = 20\%$ (blue data curve (triangles), inset (b)), i.e., with curvature radii exceeding the exchange length $l_{\text{exch}}$ by several multiples, has to be introduced in order to suppress the asymmetric vortex state. This can be seen from the fact that only for the blue curve (triangles) $\langle M_x \rangle / M_S = 0$ holds at $H_{\text{ext}} = 0\,\text{A m}^{-1}$. This stability of the asymmetric vortex state with regard to the rounding of corners is remarkable for two reasons, namely that (i) its occurrence is due to high demagnetization fields in the vicinity of sharp corners and edges,[4] and (ii) there is a general sensitivity of micromagnetic states to changes of the shape (as seen in the first part of this article).

## IV. CONCLUSION

In this article the effect of a rounding of corners and edges of ferromagnetic, pyramidal-shaped shell structures on the magnetic reversal behavior is studied on the basis of two examples. Considering the reversal of (quasi-)homogeneous states along their easy-axis direction, it is shown that the introduction of a small rounding ($r^{\text{rel}}_{\text{top}} = r^{\text{rel}}_{\text{base}} = 7.5\%$) reduces the coercivity by about a factor 2. This reduction can be explained by the fact that the rounding suppresses strong pinning fields in the vicinity of sharp corners and edges. It is also found that the symmetry of the remanent state may change, which suggests that a rounding of corners potentially leads to problems when trying to establish homogeneous configurations in soft magnetic nanostructures. The study of the magnetic reversal of the asymmetric vortex state suggests that this state may also exist in the presence of rounded corners and edges with curvature radii exceeding the exchange length by several multiples. This stability is a requirement for a potential applicability of such a state in modern memory devices.

## ACKNOWLEDGMENTS

We acknowledge funding from EU FP7/2007-2013 grant 233552.

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