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Corners and nucleation in micromagnetics¹

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Abstract

The divergence of the stray field in corners and its consequence for micromagnetic calculations was studied numerically in two dimensions for high-anisotropy materials. The results show that no atomistic theory has to be invoked because the singularity is smoothed out already within micromagnetics. The magnetic configurations and its deduced critical quantity, the coercivity, are determined correctly if the configurations are well approximated on the exchange length $\sqrt{A/K_d}$. The singularity in the stray field remains only visible in the torque balance where it is compensated by an exchange torque. © 1998 Elsevier Science B.V. All rights reserved.

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1. Introduction

In a mathematically sharp corner of a magnetic body the stray field diverges logarithmically within the continuum theory of micromagnetics [1]. Because all other fields are finite, torque equilibrium for the corner moment appears to be possible only for symmetric orientations of the magnetization (Fig. 1). According to this reasoning, the switching field of particles with corners might even be larger than that of smooth bodies. Previous numerical calculations for cubic geometries [2,3] had usually found a considerable reduction of the switching field compared to the analytically known value for ellipsoids, but the influence of sharp corners has not been studied in detail. Because the stray-field singularity can only be represented by an infinitely fine meshing in the corners, finite element results might be strongly dependent on the degree of discretization. Aharoni [4] suggested that the atomic lattice constant might have to be taken into account within micromagnetics, for this reason.

In this work we will show that the diverging stray field is effectively smoothed by the exchange stiffness term on a length scale $\sqrt{A/K_d}$ (A = exchange constant, $K_d = J_s^2/2\mu_0$ = stray-field

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Fig. 1. Possible magnetization configurations in a two-dimensional corner which keep the balance between the diverging stray-field torques.

energy constant). Because this length is for all common materials still markedly larger than atomic distances, we find that atomic lattice effects can be disregarded in the micromagnetic analysis of corners.

2. Numerical techniques and basic results

The magnetization configuration in a corner can be studied in two dimensions for high-anisotropy materials. If a magnetization parallel to the third dimension is disfavored, the balance of the two competing singular stray field components in the corner could lock the magnetization in the bisectrix. We explore this problem by numerical experiments in 2D employing the procedures of [5,6]. An infinitely extended prism with a 40×40 nm cross



Fig. 2. Magnetization profiles along the right half of the top edge in a cross section. These profiles for a field just before switching are compared for different numbers of discretization cells N along x. The curves are offset with respect to each other because they differ very little.

section and a transverse easy axis was investigated. The material parameter of NdFeB $Q = K_u/K_d =$ 4.17 (K_u = uniaxial anisotropy constant) was primarily employed. In reduced units the prism is $14.6\sqrt{A/K_d}$ wide. Starting from saturation along the easy axis, the approach to the switching instability in an opposite field was calculated for different discretizations.

In Fig. 2 we show the m_y -component of the magnetization on the upper right half of the prism just before switching. The strongest excursion prior to switching of any magnetic moment occurs in the corners. In contrast to the expected influence of the stray-field singularity, the switching mode appears independent of the discretization once the



Fig. 3. Effect of increasing discretization on the torques due to different energy terms for the neighborhood of the corner at zero field (a) and close to switching (b).

discretization cells are smaller than the exchange length. Somehow the influence of the singularity disappears in micromagnetics even when the magnetization in the corner does not point to the diagonal ($m_y = 0.81$ in the corner instead of 0.707).

3. Torque balance in the corner

To find out what happens to the infinity in the demagnetizing torques, the contributions to the total torque $m \times H_{eff}$ are plotted in Fig. 3 for the right half of the top surface for different discretizations. As expected, a better discretization leads to a better representation of the diverging demagnetizing torque in the corner. However, this divergence is balanced by an equally diverging exchange torque. The combination of external field and anisotropy torques appears largely unaffected by the discretization. Obviously, only subtle deflections in the magnetization vectors are responsible for the balancing exchange torques because they are not visible, neither in the magnetization profiles (Fig. 2) nor in the anisotropy torque contribution (Fig. 3).

4. Influence of the stray-field singularity on the switching field

Next, we address the question whether the switching process is influenced by the stray-field

singularity. To calculate the instability point of the micromagnetic configuration in a proper way we focus on the point of the strongest excursion when approaching the switching field. In the example of Fig. 2 this is the magnetization vector in the corner. The derivative of this magnetization angle with respect to the applied field diverges at the critical point. The critical field results from extrapolating the square of the inverse susceptibility to zero as shown in Fig. 4.

We find that the switching field is in fact virtually independent of the discretization for $N \ge 32$ in this example. For N = 32 one discretization cell measures $0.456\sqrt{A/K_d}$. This means that at least two discretization points within an exchange length $\sqrt{A/K_d}$ are needed to calculate the switching field in a valid way. Fig. 4b, where the switching field is plotted as a function of cell size for different *Q*values indicates that the necessary degree of discretization scales primarily with the exchange length $\sqrt{A/K_d}$.

This is demonstrated explicitly in Fig. 5, where the critical magnetization modes are plotted using two different length scales, one based on the exchange length $\sqrt{A/K_d}$, the other based on the wall width parameter $\sqrt{A/K_u}$. The results speak clearly in favor of $\sqrt{A/K_d}$ as the decisive material length in this problem. For Q = 2 a pinning of the magnetic corner moment is observed. Due to the stronger



Fig. 4. The square of the inverse susceptibility of the magnetic moment in the corner as a function of the external field for a prismatic particle with Q = 4.17 for different discretizations (a). From the extrapolation to zero the switching field H_c is derived, which is plotted as a function of discretization in (b) for different Q.



Fig. 5. Comparison of the magnetic configurations close to the critical field on the top right surface of a prismatic particle for different *Q*-values as a function of the distance from the corner measured in two alternative characteristic micromagnetic lengths.



Fig. 6. Switching fields and corner switching angles (counted from the easy axis) for the different *Q*-values.

relative importance of the stray field, the nucleation mode evolves in such a way that the strongest excursion of any magnetic moment occurs at approximately one exchange length away from the corner. It might also be noted that the moment in the corner rotates already beyond 45° . As in the case of the switching field, the critical angle can be obtained by an appropriate extrapolation (in this case a linear extrapolation of the angle versus the inverse susceptibility). The extrapolated switching fields $H_{\rm crit}$ and the switching angles for all investigated Q-values are summarized in Fig. 6.

5. Conclusions

In conclusion, we found that the diverging stray-field torques in a corner are balanced by an equally diverging exchange torque even for non-symmetrical edge magnetization directions. While the values of these torques in the finite element simulation increase with increasing discretization, this does not affect the computed switching mode and the resulting switching field as long as the discretization is finer than the exchange length. This behavior has three practical consequences:

(i) The discretization in numerical micromagnetics can ignore the logarithmic singularities in corners and edges because nature does the same.

(ii) It is not necessary to extend the discretization to the atomic level, a discretization smaller than the exchange length $\sqrt{A/K_d}$ is sufficient.

(iii) A rounding of corners in a physical microstructure is not expected to have an effect on coercivity as long as the rounding radius is small compared to the exchange length.

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