Comment on "Frustrated magnetization in Co nanowires: Competition between crystal anisotropy and demagnetization energy"

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Bergmann *et al.* [Phys. Rev. B 77, 054414 (2008)] present an analytical theory explaining the behavior of ferromagnetic cobalt nanowires with perpendicular anisotropy. This theory, which predicts a sinusoidal variation of the magnetization along the long axis of the wire, depends upon an assumption that "the magnetization is constant within a cross section of the wire." In this Comment we use micromagnetic modeling to show that this assumption does not hold in any relevant setting. For very thin wires, we show that a uniform magnetization configuration is the lowest energy state, which is consistent with some of the larger exchange stiffness results from Bergmann *et al.* For thicker wires, such as those in the referenced experimental systems, the micromagnetic simulations produce magnetization patterns containing vortices. Across all wire thickness, the sinusoidal configuration has higher energy density than the vortex configuration, and is therefore not attained. The micromagnetic simulations explain not only the periodic magnetization patterns observed in experiments, but also the occasional absence (or disappearance) of periodic structures as described in the literature.

Introduction

Bergmann *et al.*[1] consider magnetization distribution in cobalt nanowires with perpendicular anisotropy. This interest is stimulated by experiments like those described by Henry *et al.*[2] and Liu *et al.*[3], where quasiperiodic magnetization patterns are sometimes found. Let us assume that the nanowire is parallel to the z-axis and the magnetocrystalline easy axis is parallel to the x-axis. In addition to coherent magnetization oriented either in (100) or in (001), Bergmann *et al.* investigate also a *sinusoidal* state shown schematically in Fig. 1(a). They develop an analytical theory and show that for a few material constants (representative for cobalt) the sinusoidal state is energetically preferred over the coherent states. However, both the paper of Bergmann *et al.* and recent improvements by Erickson and Mills[4] are based on the assumption "when the diameter of a ferromagnetic wire is smaller than the exchange length, the direction of the magnetization is constant within a cross section of the wire" – these authors call it the "thin-wire limit"[1]. This assumption simply does not hold in nanowires of interest, where the diameter is larger than 50 nm (Ref. 2) as compared to the exchange length $\lambda = \sqrt{2A/(\mu_0 M_s^2)}$, where A is exchange constant and M_s is the saturation magnetization. λ does not exceed 7.4 nm for cobalt (for material constants see Table 1). In Ref. 1 quantitative calculations are performed for an 80 nm diameter wire only.

Using micromagnetic simulation we investigate this problem without the "thin-wire limit" assumption. We show that there are states having much lower energy than the sinusoidal state – see Fig. 2. These states, shown in Fig. 1(b) and (c) are characterized by vortex-like distributions, where the vortex core is aligned parallel to the z- or y- axes, respectively. We will call these states correspondingly *z-vortex* and *y-vortices*.

Simulation details

In this work, micromagnetic simulations were performed using the public domain OOMMF platform[5]. To account for the elongated character of the nanowires (in experiment their length often exceeds the diameter by orders of magnitude) we have applied periodic boundary conditions in the z-dimension[6]. Thus, periodicity along the wire dimension was assumed – we discuss this effect in more detail at the end of this section. We have considered different material parameters (exchange constant A, uniaxial anisotropy constants K_1 and K_2; saturation magnetization M_s was always equal to 1.38×10^6 A/m) with values similar to the previous paper[1], together with two additional cases characterized by smaller A – see Table 1. The simulation cells were cubes with edge size smaller than the exchange length. For larger simulation windows this size was up to 4 nm, while for smaller windows it went down to 1 nm. To reduce the surface discretization effect[7], the wire was always divided in the x- and y-dimensions into at least 32 cells. The energy density computation accounts for cross sectional discretization effects, and was normalized as in the previous paper[1], i.e., divided by $\mu_0 M_s / 2$.

We tested the accuracy of our simulations with the theory of Ref. 1 by performing a separate "computer experiment" with material parameters matching the ones in the first row of Table 1. Micromagnetic simulations were run using various cell sizes to check discretization effects (for review of discretization related problems see for example Ref. 8). The results are shown as points in Fig. 3. For these simulations the amplitude and period of the sinusoidal pattern were taken from the theory presented in Ref. 1 (dashed line in this figure). Unlike the other simulations in this paper, the magnetization distribution was fixed, i.e. we considered no relaxation. Bergmann *et al.* solve complex equations using Taylor series expansions. We have

repeated these calculations for our parameters (which differ slightly from Ref. 1) with additional terms; the improved result agrees quite well with our simulations using smaller cell sizes. Even with larger cells, our simulations differ from the theory by less than 0.1%.

To avoid artificial symmetries, present in simulations with periodic boundary conditions[6], we applied a random offset field with constant magnitude 0.1 mT, and the initial state for our simulations was always a random distribution. As a result, some variation in results was obtained for each set of modeling parameters.

In micromagnetic simulations one has to consider limited space – we call it the simulation window. Simulation window size in the z-direction (being the direction of applied periodic boundary conditions) impresses a periodicity on the solution. To find the natural period length for the y-vortices states, we performed a series of computations with different simulation window z-dimensions – similar to Ref. 6 (Fig. 5). The window size producing the lowest energy density is assumed to correspond to the inherent period length.

Fig. 4 shows the results of these computations for the set of material parameters found in the first row of Table 1. Note that one period contains one pair of stripes, or equivalently, two vortices. The error bars denote the difference between successive simulation window sizes. The points in Fig. 4, taken midway between the error bars, represent the period length as a function of the nanowire radius r. The period, $p(r)$, is seen to depend monotonically on r, and can be surprisingly successfully described by a simple theory where the magnetization distribution in the nanowire is compared with a so-called partial Landau-Kittel stripe domain structure in thin films[9]. Parameter α present in this theory describes the size of the magnetic x-surface charges. For details see the Appendix.

Results

Generally speaking our simulations, which seek local energy minimum, returned either a z-vortex or y-vortices state. The former was more common for thinner wires (see Fig. 2) and for smaller simulation window sizes. For larger windows more complex (and occasionally irregular) structures were found. For larger radii the core is more extended in the x-direction and approaches a Bloch domain wall configuration. See Fig. 5, where a cross section for the y-vortices state in a nanowire with larger radius is shown. Table 1 summarizes our results as compared with the theory presented in Ref. 1. Small differences in energy densities for the sinusoidal state as compared to the values in Ref. 1 (called $u_{\min}$ in Ref. 1, and as calculated by us, $u_{\sin}$) are due partly to small differences in material constants, and also because we have considered more terms in our Taylor series expansions, as described above. The second to last row in Table 1 contains no data for the sinusoidal state – this is because for those material parameters the uniform (001) state has a lower energy.

We have plotted energy density for both the z-vortex and y-vortices states as a function of nanowire radius (Fig. 2). As already seen in the $r = 40$ nm case (Table 1), both energies have similar values. For smaller radii the y-vortices state was not found – only the z-vortex state was present. Also for smaller radii the energy of the z-vortex state tends to the energy of a coherent (001) state. This is because for smaller radius only the inner part of the z-vortex state "fits" in the nanowire – actually only its core for smallest simulated case of $r = 16$ nm. For larger radii, above 128 nm, the z-vortex is not the preferred state – the energy of the y-vortices state is smaller. It should be noted, however, that another state (beside the z-vortex) appears here that also has no z-dimension dependence: a state consisting of two antiparallel z-vortices (with opposite chilarity) is slightly preferred to a single z-vortex – for sake of simplicity we do not discuss this case in more details here. From Fig. 2 we see that for smaller radii the sinusoidal state is dominated by the coherent (001) state. This is the reason why we were not able to evaluate the sinusoidal state for the second to last row in Table 1 – in that case the

analysis yields $s_{\sin} = 0$, i.e. we get a degenerated sinusoidal state equivalent to coherent (001) state.

Discussion

For all the investigated values of nanowire radius (except $r \leq 20\text{nm}$) and material constants the energy density of the z-vortex or y-vortices states was significantly lower than the energies of the sinusoidal and coherent-(001) states. This is a sign that to explain appropriately the experimental results (like those in Refs. 2, 3) one needs to abandon the "thin-wire limit" approximation used by Bergmann *et al.*[1] (repeated later in Ref. 4). Results of our simulations show that the magnetization indeed changes strongly across the nanowire cross section – except for thinner wires with radius below 20 nm. The fact that in our modeling two very different states could be produced can be explained by the quite similar energy characterizing both z-vortex and y-vortices states. This phenomenon can be also found in experiment. Ref. 2 points out that periodic structures were present only in the virgin magnetic state, and they "could not be re-observed after a magnetic field of significant amplitude was applied." This is consistent with our modeling of a nanowire of comparable diameter (75 nm for Fig. 18 in Ref. 2) where both the z-vortex and y-vortices states have similar energy, but the (non-periodic) z-vortex configuration is slightly preferred. Also, for all considered material parameters the periodicity of the y-vortices in the simulations was close to the rough experimental value of 200 nm, as reported in Ref. 2. We point out that while the much larger periodicity and end behavior found by Liu *et al.*[3] cannot be explained by the periodic y-vortices state described in this manuscript, the experimental results in Ref. 3 may be consistent with multiple z-vortex regions having aligned core directions but varying vortex chiralities. Our research is also consistent with the recent paper of Vila *et al.*, where

measurements of anisotropic magnetoresistance in cobalt nanowires suggests presence of a z-vortex state[10].

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Appendix

The magnetization distribution in the y-vortices state in a *nanowire* can be compared to the so-called partial Landau-Kittel stripe domain structure found sometimes in *thin films* (Ref. 9, page 229) – see Fig. 5. In the nanowires evaluated for this paper, magnetic y-surface charges as well as volume charges seem to be much smaller than magnetic x-surface charges. In our analysis we have defined the area of the magnetic x-surface charge to be that region where $|M_x/M_s| > ½$. Knowing the size of the x-surface charges in the z-dimension, t_z (see Fig. 5), the normalized surface charge size α, defined in Ref. 9 as $(p–t_z)/2p$, can be calculated. In the case of stripe domains, α should not depend on the film thickness; for material parameters considered here (first row in Table 1), $\alpha \approx 0.4$ – see Ref. 9, Fig. 9.2. Contrary to that, in our case a small but systematic dependence of α versus the rod radius is present – see Table 2. To avoid the details as to why in the nanowire case α depends on the wire radius (varying roughly between 0.34 and 0.4), we have simply considered two cases where α is held fixed: $\alpha = 1/3$ and $\alpha = 0.4$. In the stripe domain theory the period of the domains depends in the following way on the film thickness (we call this thickness $2r$ as we compare it with nanowire case):

$$p(r) = 2\sqrt{\frac{4\sqrt{AK_1}\,2r}{f(\alpha)4\mu_0 M_s^2/\pi^3 + 2\alpha^2 K_1}}$$

The function $f(\alpha)$ is related to an infinite sum – see equation (9.16) in Ref. 9. For $\alpha = 1/3$ its value is $f(1/3) \approx 0.292167$, whereas for $\alpha = 0.4$ we obtain $f(0.4) \approx 0.130887$. In Fig. 4, the above equation for $p(r)$ is plotted for the two selected values of α.

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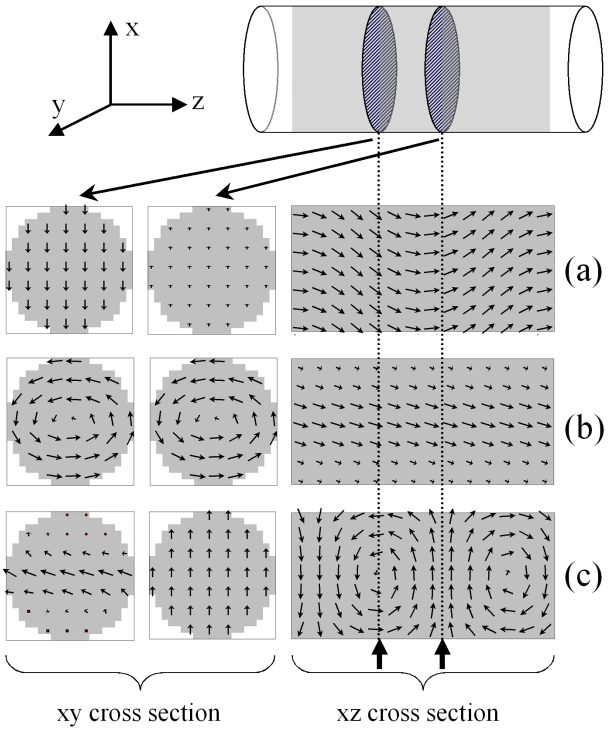

Figure 1

Figure 1. Schematic of three different magnetization states in an infinite nanowire extending along the z-dimension. xy cross sections are shown to the left, xz cross sections are shown to the right. For each case, (a), (b), and (c), we present two different xy cross sections for two different constant z-values – marked with arrows on the right side. z-vortex state (b) is z-independent, thus both presented xy cross sections are same. Bergmann *et al.*[1] investigate a *sinusoidal* state (a). However, the *z-vortex* state (b) and *y-vortices* state (c) have lower energy – see Fig. 2. Part a) is analytic theory; parts b) and c) are micromagnetic simulations.

Figure 2

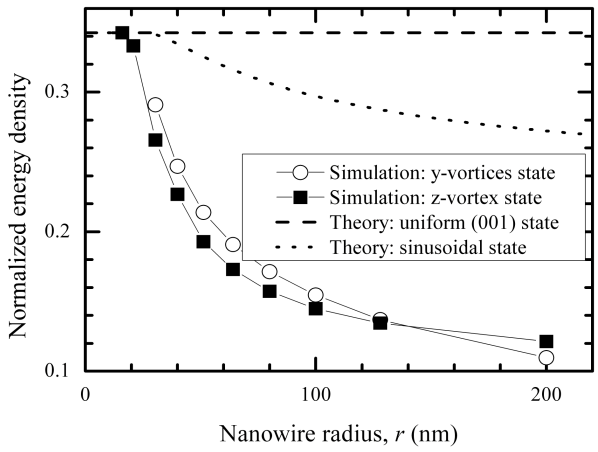

Figure 2. Energy density of the z-vortex and y-vortices structures for different nanowire radii. Results of simulations (points) are compared with theoretical values for a coherent (001) and sinusoidal state. Material constants are same as in the first row of Table 1.

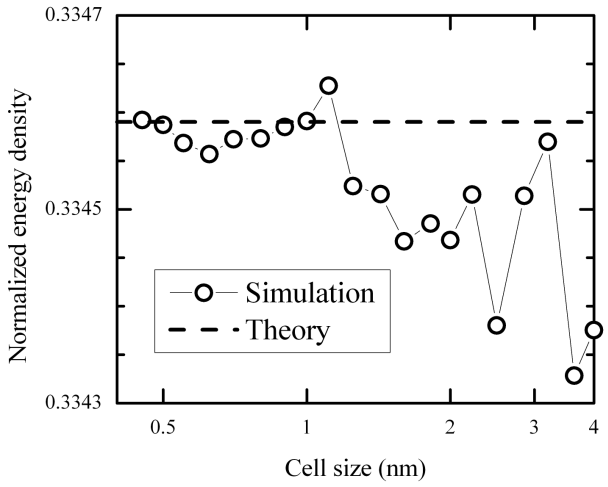

Figure 3. Normalized energy density for sinusoidal state. Dashed line – result from theory presented in Ref. 1 (material parameters: first row in Table 1). Points – micromagnetic simulations done for different cell edge sizes.

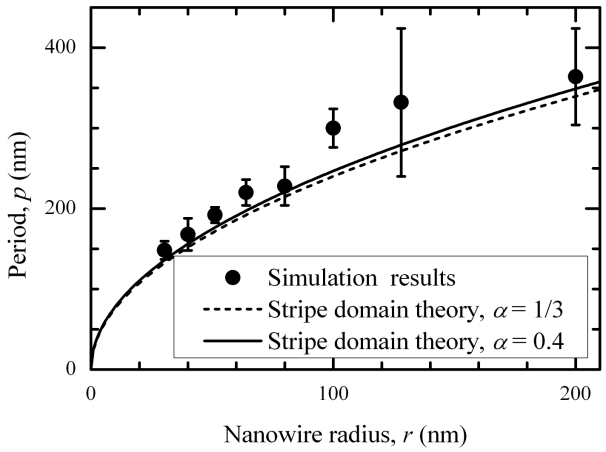

Figure 4. Periodicity of the y-vortices structure for different nanowire radii. Results of simulations (points) are compared to a simple theory, evaluated with the parameter α at two different values – see Appendix for details. Material constants are the same as in the first row of Table 1. Error bars represent the effects of simulation window z-dimension.

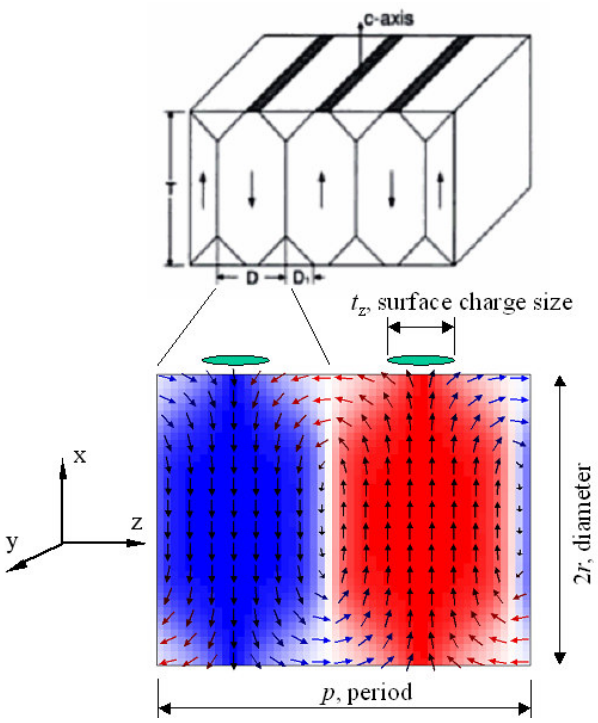

Figure 5. (Color online) Top: cross section through a structure found in thin *films* with perpendicular anisotropy. Regular domains resembling stripes are formed (from Ref. 9, page 226, Fig. 9.1(b), reproduced with permission from Cambridge University Press). Bottom: xz cross section through a simulated *nanowire* with y-vortices.

Material constants			Sinusoidal state			Uniform state	Vortex-like states		
K_1 (10^6J/m^3)	K_2 (10^6J/m^3)	A (10^{-12}J/m)	s_{sin}	θ_{sin} (rad)	u_{sin}	u_{001}	$u_{z\text{-vortex}}$	$u_{y\text{-vortices}}$	p (nm)
0.41	0	26	2.26	0.6849	0.3346	0.3426	0.2268	0.247	168
0.41	0	52	1.76	0.3212	0.3423	0.3426	0.2832	0.307	220
0.41	0.1	26	2.12	0.9555	0.3792	0.4262	0.2463	0.263	168
0.41	0.1	52	1.57	0.8499	0.3974	0.4262	0.3094	0.322	216
0.41	0.15	26	2.07	1.0251	0.3976	0.4680	0.2551	0.2701	176
0.41	0.15	52	1.52	0.9452	0.4181	0.4680	0.3213	0.323	216
0.2	0.03	13	-	-	-	0.1922	0.1274	0.148	144
0.5	0	13	2.76	1.0409	0.3692	0.4179	0.2062	0.221	150.4

Table 1. First three columns give the material constants. s_{sin}, θ_{sin}, and u_{sin} are respectively: periodicity, amplitude, and energy density minimizing the energy of the sinusoidal state, as described in Ref. 1. u_{001} is energy density of the coherent (001) state. Last three columns give the energy density for z-vortex and y-vortices states, and the periodicity of the y-vortices state. In all cases i) the nanowire radius is equal to 40 nm; ii) uniform (100) state has energy density equal to 0.5, iii) s_{sin} and all energy densities are normalized quantities, as in Ref. 1.

***r* (nm)**	30.4	40	51.2	64	80	100	128	200
α	0.34	0.35	0.37	0.37	0.38	0.40	0.40	0.40

Table 2. Dependence of normalized x-surface magnetic charges size (along z-dimension), α, versus the nanowire radius. The estimated error of α varies from 0.01 to 0.03.