Spacial Modulation of the Magnetization in Cobalt Nanowires

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Abstract

Cobalt nanowires with a diameter in the range between 50 to 100nm can be prepared as single-crystal wires with the easy axis (the c-axis) perpendicular to the wire axis. The competition between the crystal anisotropy and demagnetization energy frustrates the magnetization direction. A periodic modulation of the angle $\theta$ between $\mathbf{M}$ and the wire axis yields a lower energy.

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In recent years magnetic nanostructures have experienced a great interest in dynamic magnetic torque experiments (for ref. see for example [1]). These experiments explore the possibility to rotate the orientation of the magnetization with a current pulse. This could be an important tool in spintronics. Complementary to the dynamic experiments we want to explore the static properties of magnetic nanostructures, in particular cobalt nanowires (NW). We believe that a detailed knowledge of the static magnetic properties will have important consequences in their dynamic behavior.

A number of experimental groups [2], [3], [4], [5], [6], [7], [8], [9] have prepared Co NWs with diameters in the range of 30nm to several 100nm. Similar Co NWs with a diameter of 80nm were recently fabricated at the University
of Southern California [10]. In some of the experiments the magnetic structure of the NWs was investigated with a magnetic force microscope (MFM) [2], [8], [7], [10]. The MFM scan showed spacial oscillations of the magnetic field along the length of the wire which are sometimes quasi-periodic. Thiaville et al. [11] concluded that in their experiments the period is in agreement with a "head-to-head" magnetization, a 180° Bloch wall.

Henry at al. [7] observed by means of dark field transmission electron microscopy (TEM) images that the Co NWs have the bulk hexagonal structure. For wire diameters 2R < 50nm the easy c-axis lies parallel to the wire axis while for NWs with diameters of 2R > 50nm the easy c-axis is perpendicular to the NW axis. In the following we discuss the latter case, NWs with a diameter 2R > 50nm. Below we choose a radius of R = 40nm for quantitative calculations. We denote the wire axis as the z-direction and the easy axis as the x-direction of our coordinate system.

When the axis of the Co NW and the easy axis lie perpendicular to each other then the magnetization is frustrated. The shape or demagnetization anisotropy prefers to align the magnetization in the z-direction, parallel to the wire axis. But the crystal anisotropy definitely favors the x-direction. And this crystal anisotropy is very large in the uniaxial Co wire.

The shape or demagnetization anisotropy energy density (ED) is due to the demagnetization field and given by

\[ u_d = \frac{\mu_0}{2} \mathbf{MN} \mathbf{M} = -\frac{\mu_0}{2} \mathbf{H} \cdot \mathbf{M} \]

where \( \mathbf{N} \) is the 3x3 demagnetization matrix, \( \mathbf{H} \) is the demagnetization field, i.e. the magnetic field in the absence of an external magnetic field, and \( \mathbf{M} \) the magnetization. We introduce \( \theta \) as the angle between the z- or wire axis and the magnetization \( \mathbf{M} \). (Within this paper the magnetization will always lie in the x-z-plane). Then one has a demagnetization factor of \( N_{xx} = \frac{1}{2} \) for \( \theta = \pi/2 \) (perpendicular to the wire) and \( N_{zz} = 0 \) for \( \theta = 0 \) (parallel to the wire axis). For a constant magnetization \( \mathbf{M} = M_0 (\sin \theta, 0, \cos \theta) \) under the angle \( \theta \) the demagnetization energy density is

\[ u_d = \frac{1}{2} \sin^2 \theta \left( \frac{\mu_0}{2} M_0^2 \right) \]

We take from O’Handley [12] the reference value for the magnetic ED of Co \( u_{00} = \frac{\mu_0}{2} M_0^2 = 12 \times 10^5 J/m^3 \). The value of \( u_d/u_{00} \) is 0 for \( \mathbf{M} \) parallel to the wire axis and 1/2 for \( \mathbf{M} \) parallel to the easy axis.
The energy density of the crystal anisotropy is generally given in terms of the angle between the easy axis and the magnetization. In our geometry this angle is equal to \((\frac{\pi}{2} - \theta)\). The crystal anisotropy \(E_D\) is, in terms of this angle:

\[
uca = k_1 \cos^2 \theta + k_2 \cos^4 \theta\]

The crystal anisotropy constant \(k_1\) is given in the literature as \(k_1 = 4.1 \times 10^5 J/m^3\) \([12]\). For the constant \(k_2\) one finds different values in the literature, for example \(k_2 = 1.5 \times 10^5 J/m^3\) \([12]\) and \(k_2 = 1.0 \times 10^5 J/m^3\) \([13]\). The resulting crystal anisotropy \(E_D \nuca/\nu_{00}\) is 0.47 (0.425) along the wire axis and 0 parallel to the easy axis. (The value in parenthesis is for \(k_2 = 1.0 \times 10^5 J/m^3\).) This difference in the constant \(k_2\) has important consequences. The value of \(k_2 = 1.5 \times 10^5 J/m^3\) yields the lowest \(E_D \nuca/\nu_{00}\) = 0.450 for a finite angle of \(\theta = 0.65 \equiv 37^\circ\) between the magnetization and the wire axis. For the value of \(k_2 = 1.0 \times 10^5 J/m^3\) the magnetization would align parallel to the \(z\)-axis.

Obviously the competition between the crystal anisotropy and demagnetization is a close call. The system will try to reduce its energy as much as possible by the crystal anisotropy without paying too much energy to the demagnetization energy. One way to reduce the demagnetization energy is to modulate the magnetization direction in the \(x\)-\(z\)-plane so that the angle \(\theta\) between \(\mathbf{M}\) and \(\hat{z}\) oscillates as \(\theta = \theta_0 \cos (kz)\). (There is no oscillation in time but only in space in contrast to spin waves in NWs which have been treated by Arias and Mills \([14]\).) While for a constant magnetization in \(x\)-direction the field \(\mathbf{H}\) falls off as \(1/\rho^2\) with the distance \(\rho\) from the wire axis, a modulated magnetization with a period \(\lambda\) will cancel the field for distances \(\rho\) which are larger than \(\lambda\). This reduces the demagnetization \(E_D\). In this paper we investigate the effect of such a modulation on the \(E_D\) of the wire. This modulation corresponds to a magnetization \(\mathbf{M}\)

\[
\mathbf{M} = M_0 (\sin (\theta_0 \cos kz), 0, \cos (\theta_0 \cos kz))
\]  

(1)

In Fig.1 the orientation of the magnetization is shown as a function of \(z\). We keep the absolute value of \(|\mathbf{M}| = M_0\) constant.
The magnetization components $M_x$ and $M_z$ can be expressed as two Fourier series.

$$M_x(z) = M_0 \sum_{\nu=0}^{\infty} c_{2\nu+1} \cos[(2\nu + 1)kz]$$

$$M_z(z) = M_0 \sum_{\nu=1}^{\infty} c_{2\nu} \cos(2\nu k z)$$

The coefficients $c_{2\nu+1}, c_{2\nu}$ can be easily obtained from a Fourier expansion of $M$ in equ. (1). The lowest coefficients are $c_0(\theta_0) = \left(1 - \frac{1}{4}\theta_0^2 + \frac{1}{64}\theta_0^4 - \ldots\right)$, $c_1(\theta_0) = \left(\theta_0 - \frac{1}{8}\theta_0^3 + \frac{1}{192}\theta_0^5 - \ldots\right)$, etc. We include terms up to the order of $\theta_0^{18}$.

In the next step we calculate the demagnetization field $H$ for a magnetization $M_x = M_{x0} \cos(qz)$. Setting afterwards $q = (2\nu + 1)k$ and $M_{x0} = M_0 c_{2\nu+1}$ the results can be used for each Fourier component.

The magnetic flux $B$ inside and outside of the sample is given by $B = \mu_0 (H + M)$. Since there are no external currents in our problem the curl of the magnetic field vanishes, $\nabla \times H = 0$. Therefore the magnetic field can be expressed as the gradient of a magnetic potential $H = -\nabla \phi$ (in full analogy the electrostatic case). Taking the divergence of the magnetic flux (which vanishes) yields

$$0 = \nabla \cdot B = \mu_0 (\nabla \cdot H + \nabla \cdot M)$$

and replacing the field by the potential yields

$$\nabla \phi = \nabla \cdot M$$

For $M_x$ the divergence of $M$ is zero.

We use cylindrical coordinates ($\rho, \varphi, z$) and take the $\varphi$-dependence as $\cos \varphi$. Then the solutions of the Laplace equation are

$$\phi = \begin{cases} 
C^{\text{in}} I_1(q\rho) \cos \varphi \cos qz & \rho < R \\
C^{\text{out}} K_1(q\rho) \cos \varphi \cos qz & \rho > R 
\end{cases}$$
where $I_1(s)$ and $K_1(s)$ are modified Bessel functions. The coefficients $C^{in}, C^{out}$ are obtained by using the boundary conditions at $\rho = R$. The components $B_\rho$ and $H_\varphi$ have to be continuous. This yields $C^{in} = RM_{x0}K_1(qR)$ and $C^{out} = RM_{x0}I_1(qR)$. (In determining the coefficients one obtains the Wronski determinant $W = [I_1(qR) K'_1(qR) - I'_1(qR) K_1(qR)]$ as a denominator, which has the value $W = -1/(qR)$).

From the magnetic potential one obtains the components of the magnetic field $H$. The x-component of $H$ inside the wire is

$$H_x(\rho < R) = -qRK_1(qR) \left[I'_1(q\rho) \cos^2 \varphi + \frac{1}{q\rho} I_1(q\rho) \sin^2 \varphi \right] M_{0x} \cos(qz)$$

The local demagnetization ED is $- (\mu_0/2) H_x M_x$. We average over a period in z-direction and the cross section $\pi R^2$ and obtain for an individual Fourier component the demagnetization ED

$$\left(\frac{\mu_0}{2} M_{x0}^2\right) \frac{1}{2} K_1(qR) I_1(qR)$$

For each $q = (2\nu + 1)k$ the demagnetization field $H$ interacts only with the magnetization $M$ of the same $q$ (after averaging). Then the total contribution of all components of $M_z$ is just the sum of the individual contributions. In the following we normalize all EDs by dividing by the value $u_{00} = \frac{\mu_0}{2} M_0^2$. Then the normalized ED is

$$\frac{u_x(s, \theta)}{u_{00}} = \sum_{\nu=0}^{n} (c_{2\nu+1}(\theta))^2 \frac{1}{2} K_1[(2\nu + 1) s] I_1[(2\nu + 1) s]$$

where $s = kR$. In the numerical evaluation we include three terms (the third hardly contributes).

The Fourier components $M_z = M_{z0} \cos qz$ for the z-component of the magnetization are calculated quite analogously. The main difference is that the magnetic field $H$ and therefore the magnetic potential are independent of $\varphi$. Therefore $\phi$ is given by the modified Bessel functions $I_0(q\rho)$ and $K_0(q\rho)$ of order zero. Furthermore $\Delta \phi$ does not vanish but is given by

$$\Delta \phi = \frac{dM_z}{dz} = -M_{z0}q \sin(qz) \neq 0$$

The solution is found in complete analogy to the $M_x$-component and is given by
\[ \phi (\rho, z) = R M_{\rho 0} \sin (qz) \begin{cases} \left[ \frac{1}{qR} + K'_0 (qR) I_0 (q\rho) \right] & \rho < R \\ I'_0 (qR) K_0 (q\rho) & \rho > R \end{cases} \]

The magnetic field component \( H_z \) inside the wire is

\[ H_z (\rho < R) = - (qR K'_0 (qR) I_0 (q\rho) + 1) M_{\rho 0} \cos qz \]

In the evaluation of the demagnetization ED we use the identities \( t I_0 (t) = d (t I_1 (t)) / dt, K'_0 (t) = - K_1 (t), I'_0 (t) = I_1 (t) \). The averaged demagnetization ED becomes \( \left( \frac{\mu_0}{2} M^2 \right) \left( \frac{1}{2} - K_1 (qR) I_1 (qR) \right) \). The contribution of all Fourier components of \( M_z \) is

\[ u_z (s, \theta_0) \frac{u_{00}}{u_{00}} = \sum_{\nu=1}^{\infty} \left( c_{2\nu} (\theta) \right)^2 \left( \frac{1}{2} - K_1 (2\nu s) I_1 (2\nu s) \right) \]

Again we include the first three terms in the numerical evaluation.

Next we consider the crystal anisotropy ED. The average of the term \( k_1 \cos^2 \theta \) yields

\[ \frac{u_{ca}^{(1)} (\theta_0)}{u_{00}} = \frac{1}{u_{00}} \frac{1}{2\pi} \int_0^{2\pi} k_1 \cos^2 (\theta_0 \cos s) d (s) = 0.34 \times a_1 (\theta_0) \]

where \( a_1 (\theta_0) = 1 - \frac{1}{2} \theta_0^2 + \frac{1}{8} \theta_0^4 - +... \). The average of the term \( k_2 \cos^4 \theta \) yields

\[ \frac{u_{ca}^{(2)} (\theta_0)}{u_{00}} = 8.3 \times 10^{-2} \times a_2 (\theta_0) \]

for \( k_2 = 1.5 \times 10^5 J/m^3 \) with \( a_2 (\theta_0) = 1 - \theta_0^2 + \frac{5}{8} \theta_0^4 - +... \). In both cases we include terms up to the order of \( \theta_0^{18} \).

Finally we have to include the exchange stiffness of the Co wire. While a modulation of the magnetization can reduce the demagnetization and the crystal anisotropy energy, it will cost energy because of the bending of the magnetization. The increase in the ED can be expressed in terms of the exchange stiffness constant \( D_{ex} \)

\[ u_{ex} = \frac{1}{4 g \mu_B} \theta_0^2 D_{ex} k^2 \]

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Since the energy densities $u_x$ and $u_z$ are a function of $kR$ and $\theta_0$ we express all energies as functions of $s = kR$ and $\theta_0$. Then we obtain

$$\frac{u_{ex}}{u_{00}} = \frac{1}{4} \frac{M_0 D_{ex}}{u_{00} R^2 g \mu_B} \theta_0^2 s^2$$

Liu et al. [15] determined the exchange stiffness $D_{ex}$ experimentally from the spin-wave spectrum in hexagonal Co. They also performed a theoretical calculation. From the experiment they obtained $D_{ex} = 435 \text{meV} \times A^2 = 6.96 \times 10^{-40} \text{Jm}^2$. Their theoretical result yielded twice this value. Using the experimental value and a radius of $R = 40 \text{nm}$ we obtain $u_{ex} = 8125 \times (kR)^2 \theta_0^2 [\text{Jm}^{-3}]$. The normalized exchange stiffness ED is then

$$\frac{u_{ex}}{u_{00}} = a_{ex} s^2 \theta_0^2, \quad a_{ex} = 0.68 \times 10^{-2}$$

This exchange ED is very small compared with the demagnetization and the crystal anisotropy EDs which are of the order of 1.

Finally we add all terms and calculate the total ED as a function of $s = kR$ and $\theta_0$ and determine the minimum of this energy

$$u_t (s, \theta) = \frac{1}{u_{00}} [u_x(s, \theta_0) + u_z(s, \theta_0) + u_{ca}(\theta_0) + u_{ex}(s, \theta_0)]$$

We perform the calculation for different choices of the parameter $k_2$ and determine the position of the minimum of the ED in the $s-\theta_0$-plane. To investigate the effect of the exchange ED we also perform a calculation with twice the experimental value for $a_{ex}$. In table I the numerical results for different parameter choices are collected.

| $k_2/u_{00}$ | $a_{ex}/u_{00} \times 10^{-2}$ | $s_{min}$ | $\theta_{min}$ | $u_{min}/u_{00}$ | $u |\hat{M}||\hat{z}|$ | $u |\hat{M}||\hat{x}|$ |
|--------------|-------------------------------|-----------|----------------|------------------|-----------------|-----------------|
| 0            | 0.68                          | 2.3       | 0.7            | 0.33388          | 0.342           | .5              |
| 0.083        | 1.36                          | 1.75      | 0.3            | 0.34137          | 0.342           | .5              |
| 0.083        | 0.68                          | 2.1       | 1.0            | 0.37883          | 0.425           | .5              |
| 0.125        | 1.36                          | 1.6       | 0.8            | 0.3969           | 0.425           | .5              |
| 0.125        | 0.68                          | 2.1       | 1.0            | 0.39704          | 0.425           | .5              |

Table I: For two values of $k_2$ and $a_{ex}$ the coordinates and the value of the (normalized) energy density (ED) in the $s-\theta_0$-plane are collected in columns three, four and five. Columns six and seven give the ED for a constant magnization parallel to the z- and the x-asis.
For $k_2/u_{00} = 0.125$ and $a_{ex} = 0.68 \times 10^{-2}$ we find the minimum at $(s, \theta_0) = (2.1, 1.0)$. In Fig.2a,b the dependence of $u_t/u_{00}$ is plotted for these parameters. The figures show two orthogonal traces through the energy minimum (a) along the $s = kR$ direction and (b) along the $\theta_0$ direction.

Fig.2a,b: The ED as a function of $s = kR$ (3a) and $\theta_0$ (3b) through the minimum for the parameters $k_2/u_{00} = 0.125$ and $a_{ex}/u_{00} = 0.68 \times 10^{-2}$.

For $\theta_0 = 1.0$ we can draw the two components $M_x$ and $M_z$ as a function of $z$ along the wire. This is shown in Fig.3. With $\theta = 1.0 \cdot \cos(kz)$ the amplitude of the angle is less than $\pi/2$. Therefore the $z$-component never reverses direction. At $\sin(1.1) = 0.84$ the $x$-component reaches almost the saturation magnetization.

Fig.3a: The $x$- and the $z$-component of the magnetization as a function of position $s = kz$. 

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For a comparison we calculate the ED when the magnetization angle rotates in the x-z-plane as $\theta = \cos (kz)$. This yields

$$\mathbf{M} = M_0 (\sin (kz), 0, \cos (kz))$$

In this case we have only one Fourier component in x- and z-directions with the same wave number $k$. The demagnetization ED follows from the above calculation. (There is no cross term between the x- and z-part of the demagnetization ED since their $\varphi$-components are orthogonal). The $k_1$-part of the crystal anisotropy ED has the weight $1/2$ and the $k_2$ has a weight of $3/8$. The exchange stiffness ED is just $u_{ex}/u_{00} = 0.68 \times 10^{-2} s^2$. Fig.4 shows the dependence of the total ED $u_t/u_{00}$ as a function of $s = kR$. The total ED has its smallest value of $u_t/u_{00} = 0.4677$ at $k = 0$. This value is considerably higher than for a constant magnetization along the NW axis with $u_{||}/u_{00} = 0.408$. Therefore this behavior of the magnetization is energetically unfavorable.

![Fig.4: The total energy density for a spatial rotating magnetization as function of $s = kR$.](image_url)

Finally we want to discuss the physics of the solution and compare it with the experiment.

The numerical results yield a rather short period for the modulation, about 3 times the radius. The reason for this short period is the smallness of the exchange stiffness. The sum of the demagnetization EDs $(u_x + u_z)/u_{00}$
decreases monotonically with increasing \( s = kR \) (for constant \( \theta_0 \)). Only the exchange stiffness which increases as \( k^2 \) can limit the value for \( s \).

In the real world the modulation of the magnetization has to overcome a serious obstacle, the pinning forces in the wire. The coercitive force is a manifestation of such pinning forces. In future work we intend to determine the strength of the nucleation force for this modulation. It has to be stronger than the pinning force to achieve the periodic structure. However, there are a number of MFM images which show a quasi-period modulation of the magnetic field along the Co NW. In ref \[7\], Fig.12, two MFM images are shown of a Co NW which is touched by a short NW. The images appear to show a periodic sequence of light and dark spot (in the densimeter trace along the NW does not resolve the fine structure). In ref. \[8\] the MFM image of a Co NW with \( 2R = 35nm \) shows a quasi-periodic field. However, the ratio of period to radius is not easily extracted from these images. One particularly good example are the experiments by Belliard et al. \[2\] with [Co/Cu] NWs. For example MFM images of a multi-wire with [170nm Co/10nm Cu] appear to show opposite magnetization for neighboring segments. We expect that the demagnetization ED causes an anti-ferromagnetic coupling between neighboring Co segments.

It throws some additional light on the physics of the modulated magnetization if one applies the above considerations to a Co wire with a macroscopic radius, for example \( 2R = .8mm \). If one assumes as before a modulation of \( \theta = \theta_0 \cos (kz) \) then one obtains an optimal ED of \( u_t/u_{00} = 0.21362 \). This is about half the energy for the magnetization parallel to the wire axis. However, for a macroscopic wire one should replace the sinusoidal phase modulation by a more favorable one, close to a square wave. This will reduce the ED even further. This calculation is in progress and will be published elsewhere.

It is quite remarkable that we learn from the study of nanowires that the classical "ground state" of a macroscopic uniaxial wire is very different from what we thought it was. Of course, in the real world it will be very hard to prepare a macroscopic Co wire with sufficiently small concentration of pinning centers so that the magnetization can optimally align. Nanowires are much better suited for the observation of this modulation because they have fewer pinning centers.

Abbreviations used: NW = nanowire, ED = energy density.
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