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Orientation and Temperature Dependence of Domain Wall Properties in FePt

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An investigation of the orientation and temperature dependence of domain wall properties in FePt in presented. We use a microscopic, atomic model for the magnetic interactions within an effective, classical spin Hamiltonian constructed on the basis of spin-density functional calculations. We find a significant dependence of the domain wall width as well as the domain wall energy on the orientation of the wall with respect to the crystal lattice. Investigating the temperature dependence we demonstrate the existence of elliptical domain walls in FePt at room temperature. The consequences of our findings for a micromagnetic continuum theory are discussed.

The large value of magneto-crystalline anisotropy energy of the $L1_0$ phase of FePt makes it an ideal candidate for recording media for storage densities of 1Tb/in^2 and beyond [1]. The purpose of the current letter is to address an intriguing property of FePt, specifically arising from the nature of the $L1_0$ phase, which is a layered structure consisting of alternate Fe and Pt atomic planes. The fundamental interactions at the electronic level are strongly modified by this structure. In particular it has been shown [2] that the Fe moments can be considered as localized, while the Pt induced moments have to be treated as essentially delocalized. Nevertheless, it is possible to construct a classical spin Hamiltonian involving only the Fe degrees of freedom, with the introduction of a 2-ion anisotropy term and a modified exchange term [2]. As one might expect the exchange energy is stronger within the Fe planes. This of course poses the interesting possibility of a corresponding directional dependence of the domain wall width. This is one of the related topics forming the subject of this letter. In this context the work to be presented here has an impact on micromagnetics.

Micromagnetics is a continuum formalism used for the calculation of magnetization structures and reversal mechanisms in magnetic materials. Its basis [3] is the minimization of a total energy comprising the sum of exchange, magneto-static, anisotropy and Zeeman terms. Under the assumption of small angular changes between individual spins on neighboring atoms (corresponding to the approximation of long wavelength magnetization fluctuations) it is straightforward to show, that the exchange energy is given by

$$E_{ex} = \int \mathrm{d}^3r \, A \left(\nabla M(\mathbf{r}) \right)^2, \qquad (1)$$

where for a simple cubic lattice $A = J/2a$ with J the exchange integral and a the lattice spacing. We note that the atomic level information has become absorbed into the constant A, an approximation which is central to the micromagnetic approach which, hence, cannot render the microscopic details of exchange interactions [4]. The directionality of J clearly has important implications for micromagnetic simulations of FePt and other layered magnets.

In this letter we describe the results of atomistic calculations of the Domain Wall (DW) width in FePt, demonstrating first its directionality. Atomistic calculations are carried out using the Heisenberg form of exchange, and are free of the long-wavelength approximation inherent in micromagnetics. Thus we are able to calculate values of the constant A, including its directionality, for FePt. This is important for micromagnetic calculations of FePt and indeed all layered ferromagnets. Furthermore, the atomistic approach allows magnetization fluctuations at all wavelengths, allowing the prediction of temperature dependent magnetic properties. As a result we are able to study the temperature dependence of the DW width, which is found to be significant. Finally, we consider the nature of the DW in FePt. The normal Bloch-type DW is referred to as a circular DW since it involves a rotation of the magnetization which retains a constant magnitude. However, there exists an alternative structure, the elliptical DW, in which the magnetization decreases in magnitude during the rotation. The DW width in FePt is rather small, which is a criterion for observing elliptical DW structures [5]. In this letter we study the DW structure in FePt and demonstrate a continuous change from a circular (Bloch-type) DW at 0K to an increasingly elliptical structure with increasing temperature.

FePt is modeled in the ordered $L1_0$ phase using an effective Hamiltonian for classical spins $\mathbf{S}_i$ with magnetic moment μ and $|\mathbf{S}_i| = 1$. This model [2] has been constructed on the basis of first-principles calculations of non-collinear configurations calculated using constrained local spin density functional theory [6] and site-resolved magneto-crystalline anisotropy[7]. It is used here to investigate the domain wall properties of FePt. The full Hamiltonian, as described in Ref. [2], including the cou-

pling to a magnetic field $\mathbf{B}$ and dipole-dipole coupling, is,

$$\mathcal{H} = -\sum_{i<j} \left(J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j + d_{ij}^{(2)} S_i^z S_j^z \right) - \sum_i d^{(0)} (S_i^z)^2$$
$$- \sum_{i<j} \frac{\mu_0 \mu^2}{4\pi} \frac{3(\mathbf{S}_i \cdot \mathbf{e}_{ij})(\mathbf{e}_{ij} \cdot \mathbf{S}_j) - \mathbf{S}_i \cdot \mathbf{S}_j}{r_{ij}^3} - \sum_i \mu \mathbf{B} \cdot \mathbf{S}_i, \quad (2)$$

where the two-ion anisotropy parameters $d_{ij}^{(2)}$ are the dominant contribution to the uniaxial anisotropy energy in relation to the single-ion term $d^{(0)}$. Interestingly, the exchange interactions J_{ij} depend on the orientation in the crystal. Fe-Fe exchange interactions within the Fe planes are stronger than those perpendicular to the planes via the Pt sites. As we will show in the following, this fact will lead to unusual domain wall properties.

Since we are interested in ground state properties as well as finite temperatures we use Langevin dynamics, i. e., simulations of the Landau-Lifshitz-Gilbert equation of motion with the dimensionless Gilbert damping parameter $\alpha = 1$. We assume that a possible temperature dependence of our effective spin model is sufficiently weak to be neglected in the temperature range we are interested in. Thermal fluctuations are included as an additional noise term in the internal fields which fulfils the fluctuation-dissipation theorem. The value of α as well as the form of the damping and noise will not influence our results because we are solely interested in equilibrium properties rather than the dynamics of the system. All algorithms we use are described in detail in [8]. Using these methods we are able to calculate thermal properties in models with up to 5×10^5 spins including short-range magnetic correlations.

We have applied the atomistic model outlined above to calculations of DW structures in FePt. We use a computational cell with cubic shape in zero external field heating up from 0K to above room temperature. We force a DW into the system by using fixed, anti-parallel boundary conditions for two opposite planes and open boundary conditions otherwise. Since we are interested in effects caused by the orientation of a DW, two orientations are considered, where the domain walls are either perpendicular ($\perp$) or parallel ($\parallel$) to the Fe-planes (shown schematically in Fig. 1). In the following we show only results for the largest systems we simulated with a cross section of $25.6 \times 25.6 \text{nm}^2$ and a length of 12.8nm, which was found sufficiently large to avoid finite size effects.

Calculated wall profiles were found to be well described by the usual equations [5],

$$m_t(T) = h_t(T) \cosh^{-1}\left(\pi x / \delta(T) \right) \quad (3)$$
$$m_z(T) = h_z(T) \tanh\left(\pi x / \delta(T) \right), \quad (4)$$

where h_t and h_z are the amplitudes of the magnetization and δ is the DW width. At 0K one finds a perfect circular Bloch wall with widths parallel and perpendicular to the

Fe layer of 3.7 and 4.8nm respectively; a directionality of around 30%.

With increasing temperature the DW widths increase and the shape of the domain walls changes to elliptical. As an example Fig. 2 shows the easy (z) as well as the transverse (t) component of the magnetization at 311K. The reduced maximum of the transverse component (relative to the saturation magnetization) is the signature of an elliptical wall. In order to investigate these effects in more detail we fitted the simulated DW profiles to Eqs. 3 and 4 and with that determined the amplitudes as well as the DW widths (both shown in Fig. 3).

Since exchange interactions within the Fe-planes are larger than those perpendicular to the Fe-planes, domain walls with an orientation perpendicular to the Fe-planes have a larger energy contribution from exchange and, hence, are wider. While the orientation has an influence on the DW width, it has no significant effect on the shape of the walls as one can see in Figs. 2. In all cases there is a good fit to the tanh- profile. With increasing temperatures though, the DW widths increase and the shape of the domain walls changes to elliptical. It is amazing that already at room temperature elliptical domain walls can be found with an ellipticity of at least 10%. This fact is due to very small DW widths found in FePt because of its enormous anisotropy [5].

In the following we investigate in how far our findings affect the energy of the domain walls. Therefore, we calculate DW energies from energy differences between systems with and without DW. We focus on these differences for the total energy $\Delta E/J$, the exchange energy $\Delta E_{ex}/J$, and the anisotropy energy $\Delta E_a/J$ (the sum of single-ion and two-ion anisotropy contributions). The contribution of the dipolar energy — even though taken into account — is rather small and not shown in the following. All DW energies are densities (per cross sectional area counted in number of atoms) and in units of $J = \sum_j J_{ij} = 3.52 \times 10^{-20}$J, the sum over all exchange interactions per Fe atom. In Fig. 4 these energy differences ΔE are shown versus temperature for both of the orientations of the DW.

The total DW energy $\Delta E/J$ for a wall with perpendicular orientation is about 25% higher than that for a wall with parallel orientation. This remarkable effect is once again due to the fact that exchange interactions within the Fe-planes are larger than those perpendicular to the Fe-planes. Hence, the energy is larger in perpendicular walls. Since, as a consequence, perpendicular walls are wider the anisotropy energy stored in a DW increases as well. Furthermore, the total energy increases with increasing temperatures. The exchange energy contribution $\Delta E_{ex}/J$ shows an equivalent behavior, while the anisotropy $\Delta E_a/J$ diminishes.

Using calculated values for the DW energy and width we calculate corresponding materials parameters of a micromagnetic continuum theory. However, due to the ori-

entation dependence of the DW properties in this layered ferromagnet different exchange parameters have to be taken into account for different directions. Using the equations $\delta_l = \pi\sqrt{A_l/K_l}$, and $\Delta E_l = 4\sqrt{A_l K_l}$, with $l = \perp, \parallel$ we can estimate the (anisotropic!) micromagnetic exchange parameters $A_\perp$ for the x and y components of a Cartesian coordinate system and $A_\parallel$ for the z (easy axis) component. These values differ by a factor of 1.6 while the value of the uniaxial anisotropy parameter hardly depends on the wall orientation. The corresponding numerical values are collected in Tab. I.

In summary we have carried out a study of the DW structure in FePt, which has a number of intriguing features due to the nature of the $L1_0$ phase. Firstly we predict a directionality of DW properties and their temperature dependence; the walls being wider perpendicular to the Fe planes. This reflects the directionality of the exchange interactions in FePt. The directionality of the DW width and energy is an important factor which will effect other experimental properties, such as the domain wall mobility [9–11], magneto-resistance [12], switching fields and switching modes. Furthermore, it should be considered in micromagnetic calculations on FePt (and other layered magnets). We have calculated the effective micromagnetic parameters A and K, including their directionality. K is found to be essentially independent of direction, and the range of values which we obtain for K is consistent with the large anisotropy energy of FePt (about $8 \times 10^6 \mathrm{J/m^3}$ corresponding to a zero temperature Stoner-Wohlfarth coercive field of about 16T [2]). The value for A is also consistent with the Curie temperature of FePt (a Curie temperature of about 700K corresponds to an exchange constant of about $2 \times 10^{-11} \mathrm{J/m}$). Remarkably, we also find a transition to elliptical DW structures at finite temperatures. This is due to the high anisotropy of FePt and, importantly, suggests FePt as a realistic candidate for the experimental observation of elliptical or even linear domain walls. A more detailed study of the thermodynamic behavior of domain walls in FePt, including the thermal scaling behavior of the micromagnetic exchange parameter [13] and its critical behavior, will follow.

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TABLE I: DW energy densities as well as wall widths at zero temperature, and corresponding micromagnetic exchange and anisotropy constants for perpendicular and parallel walls.

	$\Delta E/J$	δ[nm]	A [J/m]	K [J/m^3]
($\parallel$)	0.047	3.7	$1.32 \cdot 10^{-11}$	$9.35 \cdot 10^6$
($\perp$)	0.059	4.8	$2.13 \cdot 10^{-11}$	$9.27 \cdot 10^6$

FIG. 1: Sketches of the DW orientations with respect to the crystal lattice. Note, that spins rotate in the zy-plane.

FIG. 2: Easy-axis and transverse component of the magnetization vs. space coordinate for perpendicular and parallel DWs at $311K$. The solid lines represent fitted tanh- and cosh-profiles (Eqs. 3 and 4.)

FIG. 3: DW widths δ and amplitudes h versus temperature for the two different orientations of the DW.

FIG. 4: DW energy versus temperature for the two different orientations of the DW.