# Micromagnetic simulation of small-angle neutron scattering from magnetic recording media

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(Presented on 1 November 2005; published online 27 April 2006)

A micromagnetic simulation of the magnetic morphology of CoCrPtB based longitudinal recording media is used to model small-angle neutron scattering data and provide a quantitative description of the local flux density in these nanostructured magnetic materials. The model addresses several aspects of the experimental measurements and, in particular, explains an unusual increase in scattering along the applied field direction for certain values of the scattering vector **q**. The increased scattering along the field direction results in a change of the phase of the angular variation of the scattering by 90°. This 90° change in scattering phase arises naturally from the influence of stray fields when modeling the media as a heterogeneous alloy consisting of grains with a high saturation magnetization core and a permeable shell. 
[DOI: 10.1063/1.2176314]

## INTRODUCTION

In studies of nanostructured materials small-angle neutron scattering (SANS) is a very powerful technique for probing local magnetic properties. Scattering due to magnetic flux density can be separated from that due to nuclear potentials by manipulating the magnetic state of the material, for example, by applying a magnetic field so that the magnetic scattering changes while the nuclear scattering remains constant. SANS can provide information on the dimensions of changes in flux density, such as those due to granular or ordered nanoscopic particles, and it can also reveal information on the orientation of the local magnetization vector.[1–4] This is achieved via examination of the scattered neutron intensity as a function of azimuthal angle $\theta$ in the scattering plane (for SANS this is perpendicular to the incoming beam), which in our geometry is the easy plane of magnetization and parallel to the film surface. Due to the moment orientation factor in the scattering cross section $[\hat{\mathbf{q}}(\hat{\mathbf{q}}\cdot\hat{\mathbf{m}})-\hat{\mathbf{m}}]$, where $\hat{\mathbf{q}}$ is the momentum transfer unit vector and $\hat{\mathbf{m}}$ is a unit local magnetization vector, magnetic scattering falls to zero as $\hat{\mathbf{q}}$ approaches $\hat{\mathbf{m}}$. For instance, if a sample is uniformly magnetized (e.g., by applying a large external field) the scattering intensity will have an *anisotropic* dependence $I(\theta)\sim\sin^2\theta$, in which the direction of zero intensity will correspond to the orientation of the magnetization within the sample. The **q** dependence of this anisotropic scattering thus gives information on the orientation and spatial variation of the moments, in contrast to magnetometry measurements where this information is lost due to averaging over the volume of the sample. For the experimental configuration discussed here, we can reconstruct the local magnetic structure down to feature sizes of around 1 nm. Recently SANS measurements were reported on CoCrPtB longitudinal recording media sample that displays some intriguing characteristics.[3,5] The data showed that even with the application of a large external field ($H_a > H_k \sim 1.0$ T) in the plane of the sample, over certain $q$ ranges, the angular-dependent scattering intensity changed its phase $\phi$ from 0° to 90°. Here the scattering intensity is given by $I(\theta)\sim\sin^2(\theta+\phi)$, and $H_k$ is the anisotropy field. The existence of the 90° phase would seem to indicate that in these $q$ ranges there is a significant influence on the scattering from moments that are noncollinear with the applied field. The 90° phase change was found for three different fields above $H_k$. However, for fields greater than 2.2 T only the 0° phase was observed over the entire $q$ range (0.005–0.3 Å$^{-1}$). In addition to the appearance of the 90° phase shift, the data also indicated that the local intragranular magnetization has structure. This structure consists of a hard magnetic core which is significantly smaller than the physical grain size and an outer shell of weaker magnetization.[3,5] These observations challenge the view that magnetic grains in the medium are single domains of size comparable to the physical grains.

The phenomenon of scattering with 90° phase shifts of $I(\theta)$ has been observed in other systems.[1–3] In the case of

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monodispersed 10 nm Fe particles[1] the change in phase was observed at low fields and dominated the whole $q$ range. An increase in the field led to the recovery of the 0° dependence. The effect was attributed to the existence of an antiferromagnetic phase, thought to result from an oxide layer postulated to form during the fabrication process. A similar result has been also observed recently by Ijiri *et al.*[2] In this case partially oxidized iron nanoparticles have also shown 90° phase shifts. The effect was not observed over the entire $q$ range and could be also manipulated by varying the temperature and magnetic field.

Here we report the simulations of SANS data which show the possibility of a 90° phase dependence of scattering in a granular system of ferromagnetic particles with a modest size distribution (ca. 30%). In comparison to the previously reported results, we demonstrate that the origin of the phase shifts lies in the intragranular magnetic structure and is due to stray fields generated by high saturation magnetization cores at the center of the grains. To illustrate this, we compare the results of simulation with the experimental data obtained on a sample of CoCrPtB longitudinal media. This is a quantitative description of this important signature in the neutron scattering for any material system.

## MODEL

In our model the thin film medium is composed of particles (grains), with a Gaussian size distribution, close packed within a single magnetic layer. The particle separation (~12 nm) is approximately equal to the dimensions identified from transmission electron microscopy (TEM) imaging. Using the information from SANS experiments,[3,5] that is, grains are comprised of a central core surrounded by a region of weaker magnetization, we assume that the core occupies a certain fraction of the volume of the grain, with a maximum diameter equal to that of the grain itself. The cores are ferromagnetic, with a strong exchange coupling between moments in the interior of the core. The magnetic anisotropy is taken as uniaxial for each grain, with a random distribution of the principle axis in the plane of the sample. Calculation of the magnetic scattering intensity is performed using the standard Born approximation formalism[6,7] as applied to SANS experiments. The sample plane $(\hat{\mathbf{x}},\hat{\mathbf{y}})$ is positioned perpendicular to the incoming neutron beam, the external magnetic field is applied along the $\hat{\mathbf{x}}$ direction, and the scattering intensity is calculated as a function of momentum transfer vector $\boldsymbol{q}$ in the plane $(\hat{\mathbf{x}},\hat{\mathbf{y}})$ via

$$I(\mathbf{q}) \sim \frac{d\sigma_{\text{mag}}(\mathbf{q})}{d\Omega} = \left| \sum_j l_{\text{mag}} M_j(q)[\hat{\mathbf{q}}(\hat{\mathbf{q}}\cdot\hat{\mathbf{m}}) - \hat{\mathbf{m}}]\exp(i\mathbf{q}\cdot\mathbf{r}_j) \right|^2 / V. \quad (1)$$

Here, $l_{\text{mag}}$ is a constant related to the magnetic scattering potential; $M_j(q)=|\mathbf{M}_j(\mathbf{q})|=|\int \mathbf{M}_j(\mathbf{r}-\mathbf{r}_j)\exp(i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}_j))d\mathbf{r}|$ is the magnitude of the Fourier component of the magnetization vector, where $\mathbf{M}_j(\mathbf{r})$ is the magnetisation of the unit cell $j$ with the position vector $\mathbf{r}_j$; $\hat{\mathbf{m}}$ and $\hat{\mathbf{q}}$ are the unit vectors parallel to $\mathbf{M}_j(\mathbf{r})$ and $\mathbf{q}$, and $V$ is the magnetic volume.

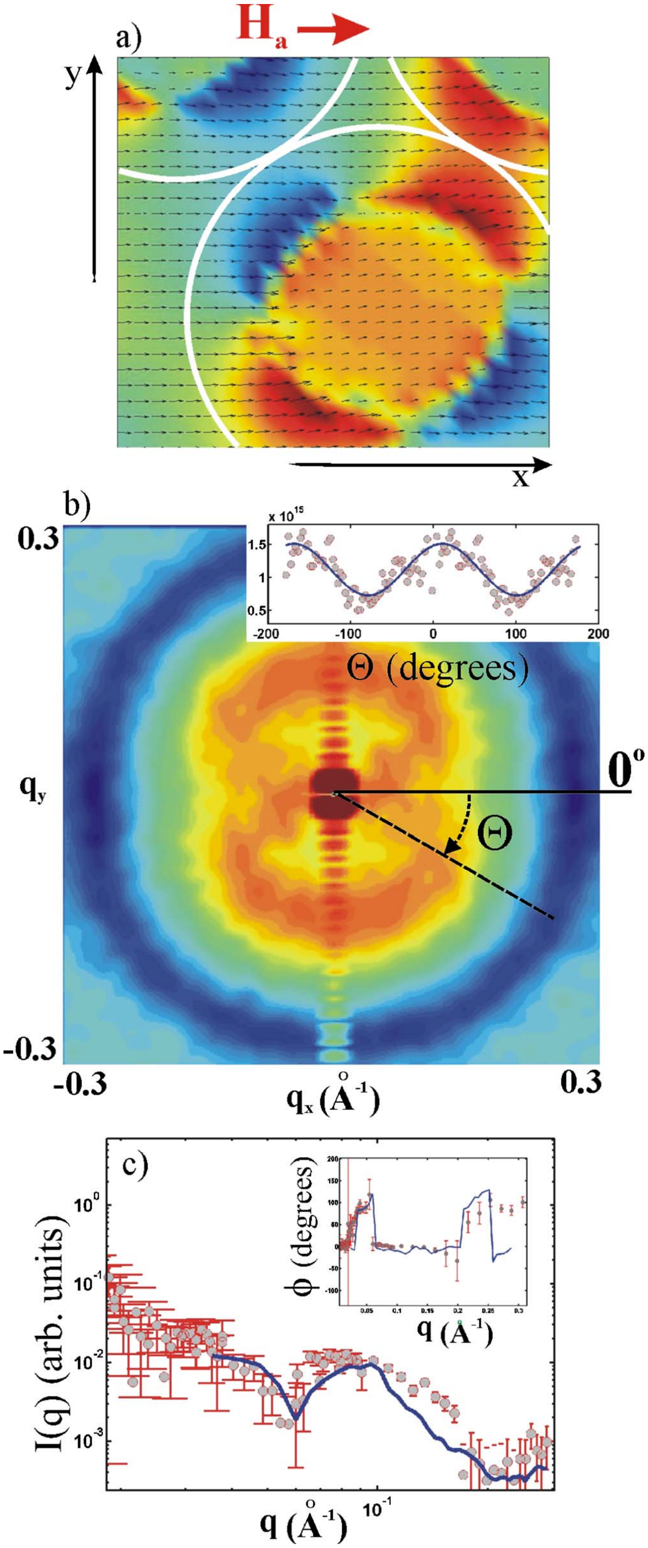


FIG. 1. (Color online) Simulation of magnetic scattering from a longitudinal medium for the case of $H_a=1.45$ T. Model parameters: Average diameter of particle core, 45 Å; particle separation, 130 Å; saturation magnetization, $M_s=500\times10^3$ A/m; exchange stiffness constant, $A=30\times10^{-12}$ J/m; anisotropy constant, $K_1=410\times10^3$ J/m$^3$. (a) Simulated magnetic flux density distribution inside and outside the cores. Color demonstrates the variation of $y$ component of **B**. White solid lines indicate grain boundaries. (b) Calculated magnetic scattering intensity $I(\mathbf{q})$ from magnetic flux density distribution shown in (a). Inset shows a 90° phase dependence of $I(\theta)$ at $q=0.05$ Å$^{-1}$. (c) Experimental and simulated dependence of the amplitude of the magnetic scattering $I(\theta)$ as a function of $q$. Inset: Experimental and calculated dependence of the phase $\phi(q)$.

In the calculation, the medium is represented by a rectangular three dimensional (3D) $(200\times 200\times 10)$ mesh of cells which contain magnetization vectors (one vector per cell). The dimension of a cell is $3\times 3\times 3$ Å$^3$. The magnitude and the orientation of $\mathbf{M}_j(\mathbf{r})$ depend on its position. For cells inside the core region, the magnetization is formed by the "spontaneous" moments in the core. These moments are tightly bound by strong exchange coupling, which keep them oriented around the same direction determined by the local uniaxial anisotropy and the direction of the internal field. In the cells outside the core region, the magnetization is formed as a result of the magnetic polarization of the material by the external applied field and the dipolar return field generated by the moments in the cores. Thus the grains in the longitudinal medium can be viewed as a two-phase system, in which one phase is represented by the hard ferromagnetic core region and the other by the surrounding soft paramagnetic-like "shell." In the simplest model, the simulation of the shell is achieved by including a linear magnetic susceptibility for the outer region such that the magnetization around the cores can be then described by the following relation:

$$\mathbf{M}_{\text{ext}} = (\mathbf{H}_D + \mathbf{H}_a)\chi, \tag{2}$$

where $\mathbf{H}_a$ is the external applied field, and $\mathbf{H}_D$ is the dipolar stray field from the moments in the cores. This allows the experimental data to be simulated with surprising accuracy over a wide range of $q$ values and applied fields. The number of particles in our simulation depends on the physical dimensions of the grains, but normally lies in the region from 40 to 60. The calculation of the flux density is performed with the OOMMF micromagnetic simulation program using the parameters given in the caption of Fig. 1. In order to account for the statistical distribution, the scattering calculation is averaged for 15 different configurations.

## DISCUSSION

The essential element of this model is that the magnetic scattering is assumed to originate from the spatial variations of all the contributions to the local flux density to which the neutron is sensitive. This includes contributions not only from the cores of the grains, but also from the magnetic material between the cores that is influenced by the long range dipolar fields. Simulations using this model not only predict the correct variation of the phase of the scattering as a function of $q$, but they also explain quantitatively the evolution of the phase shift pattern as a function of external applied field.

Figure 1 gives the experimental result obtained for a sample of CoCrPtB media measured in an applied field of 1.45 T at room temperature; the result of a simulation based on the above model is also shown. Figure 1(a) shows a simulation of the local flux density inside and around the cores. This demonstrates the dipolar nature of the stray field, which leads to a spatial variation of the $y$ component of the flux density, and which is essentially responsible for the scattering along the external field direction. Note that the $x$ components, which still dominate in real space, have Fourier components that are not significant in this $q$ range and thus do not significantly contribute to the scattering. Figure 1(b) shows the calculated two dimensional (2D) scattering image in the plane $(\hat{\mathbf{x}},\hat{\mathbf{y}})$ and the angle dependence of $I(\theta)$ which follows a $\sin^2(\theta+90^\circ)$ dependence. The amplitude of this dependence is essentially the difference between the contribution to the magnetic scattering from the $y$ and $x$ components of the local field density at the chosen $q$ value. Measuring the amplitude as a function of $q$ gives spatial information about the variations of these components on various length scales. Figure 1(c) contains the experimental and calculated results of $I(q)$. Although the simulated curve does not follow experimental data precisely, which is mainly due to simplifications in the model (e.g., the grain size variation was obtained by Gaussian distribution rather than the more usual lognormal distribution; finite size effects also play a role), the main features of the dependence are well accounted and in very good agreement with the $q$ dependence of the phase $\phi$. The inset shows the corresponding dependence of the phase as a function of $q$. These results are also in very good accord with the analytical calculations produced earlier for the same experimental data.[3]

## CONCLUSION

We have demonstrated that the shift from 0° to 90° in the phase of the anisotropic magnetic SANS data, for a field applied in the scattering plane, can be explained by the contribution to the total flux density from a permeable matrix surrounding the cores of the grains when it is influenced by the stray dipolar fields from the cores. We introduced a model which takes into account the overall variations of the flux density in a sample and which calculates the magnetic scattering for the configuration of a SANS experiment. As an example we used experimental results from longitudinal CoCrPtB media, which were simulated using the model. It was shown that in order to obtain a reasonable fit to the data the model must have (i) a significantly reduced diameter of magnetic cores and (ii) there must exist a permeable magnetic medium around the cores of the particles.

## ACKNOWLEDGMENTS

The authors would like to acknowledge the support from the University of Exeter Research Fund. We would also like to acknowledge Dr. J. Rowe for help in optimizing the programming code.

[1]J. F. Loffler *et al.*, Physica B **234–236**, 1005 (1997).
[2]Y. Ijiri *et al.*, Appl. Phys. Lett. **86**, 243102 (2005).
[3]S. L. Lee *et al.*, Mater. Res. Soc. Symp. Proc. **803**, GG4.4.1 (2004).
[4]T. Thomson *et al.*, Phys. Rev. B **72**, 064441 (2005).
[5]M. Wismayer *et al.* (in preparation).
[6]*Treatise on Materials and Technology*, edited by G. Kostorz (Academic, New York, 1979), Vol. 15.
[7]J. Weissmuller *et al.*, J. Res. Natl. Inst. Stand. Technol. **104**, 261 (1999).