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Simulation of domain formation and domain coarsening in antiferromagnetic multilayers

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Abstract

A Monte Carlo simulation of patch-domain formation and domain coarsening in antiferromagnetically coupled compensated multilayers with fourfold in-plane anisotropy is presented. The simulation accounts for both the emergence of small patch domains on unsaturation and the domain coarsening on spin flop. The autocorrelation function of the simulated domain pattern is in good agreement with published Kerr microscopic images.

Keywords: Domain growth; Domain pattern variations; Multilayers; Magnetic coupling—antiferromagnetic

Magnetic multilayers have been for a long time in the focus of interest due to their novel material properties and diverse possible technological applications. The antiferromagnetically (AF) coupled Fe/Cr system, for example, shows the giant magnetoresistance (GMR) effect [1]. The GMR noise can be influenced by the domain-size distribution of the multilayer [2]. The theoretically predicted [3] bulk spin-flop transition was first verified experimentally on a strongly AF-coupled Fe/Cr epitaxial multilayer (superlattice, SL) with fourfold in-plane anisotropy by Temst et al. [4]. Recently, on an equivalent Fe/Cr system, a reproducible domain-size-switching mechanism (domain-size coarsening at the spin-flop transition) was found by off-specular Synchrotron Mössbauer Reflectometry (SMR) and was verified by Polarised Neutron Reflectometry (PNR) [5]. In the present paper, a simple phenomenological model and results of Monte Carlo simulations of the domain-nucleation process and the domain coarsening in a magnetic SL are presented. The studied AF-coupled SL has even number of magnetic layers of equal thickness. The external field is applied along one of the two, mutually perpendicular easy axes. Two critical regions of the domain formation are investigated: (a) the 'unsaturation' region, when decreasing the field from saturation and (b) the spin-flop region when an increasing field parallel/antiparallel to the layer magnetisations results in a bulk spin-flop of the multilayer [4,6].

In a strongly AF-coupled metallic multilayer, the domain structure of the individual ferromagnetic layers is rather strictly correlated through the multilayer stack from the substrate to the surface allowing for a two-dimensional representation, e.g. by the domains of the topmost magnetic layer. In the cited SMR and PNR experiments, the investigated multilayer (MgO(0 0 1)/[^{57}Fe(26 Å)/Cr(13 Å)]$_{20}$), had a saturation field of approximately 700 kA m^{-1} [5,6]. In such a strongly coupled multilayer, the unsaturation domain formation is governed by the AF coupling and results in a characteristic patch-domain pattern in remanence [7]. This state will be called, henceforth, the primary domain state (PDS) of the multilayer. A so-called secondary domain state (SDS) is characteristic of a sample which has passed the spin-flop transition (in our particular case at approximately 10 kA m^{-1} [6]) following a saturation. In the SDS, majority large and minority small domains were observed [5]. In our model [5], we associate the domain formation and coarsening with the correlation length of the saturation field and that of the spin-flop field, being related to the unavoidable variation of the thickness of Cr spacer and the Fe layers, respectively.

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We assume the absolute thickness variations of Cr and Fe to be equivalent. Due to the strong oscillatory thickness dependence of the coupling in the Fe–Cr system [8], the actual correlation length of the AF coupling, consequently that of the 'unsaturation' domains is much smaller than the correlation length of the Cr spacer thickness. Indeed, the Fe anisotropy energy is linearly dependent on the iron layer thickness, thus the correlation length of the anisotropy energy is equal to the correlation length of the Cr spacer thickness. The spin-flop field is, however, proportional to the geometrical mean of the AF coupling and the anisotropy energy. Its autocorrelation function is, therefore, a linear combination of the autocorrelation function of the coupling and that of the spacer thickness thereby resulting in both short-range and long-range correlations [5]. Still, for clarity, we shall only use the dominant (bigger) correlation length for the spin-flop field in the present simulations.

The multilayer is modelled here by a two-dimensional grid of pixels where the colour (grey scale gradation in the figures) of each pixel represents the direction of the magnetisation of the topmost layer in a given pixel area. The mesh size of the grid (of the order of 0.1 μm) is smaller than the actual domain size (see below) but in our model, each pixel possesses a macroscopic 'classical' magnetisation, saturation field and anisotropy energy.

The primary and secondary domains are formed on this grid by first-neighbour rules explained later (see Fig. 1). Domains are represented as contiguous sets of pixels of the same colour.

The 'unsaturation' or primary domain formation is governed by the distribution of the saturation field. The higher the saturation field of a given pixel is, the sooner the pixel unsaturates. First, we create a grid of uncorrelated random numbers $U(\vec{r})$ of Gaussian distribution, where $\vec{r} = (x, y)$ is the position vector [9]. The saturation field distribution $D(\vec{r})$ is generated by smoothing the grid by an empirical width w according to

$$D(\vec{r}) = \sum_{|\vec{r}-\vec{r}'|<w} \left(1 - \frac{(\vec{r}-\vec{r}')^2}{w^2}\right) U(\vec{r}'). \quad (1)$$

Periodic boundary conditions are used. Decreasing the external magnetic field H_{ext}—along an easy axis—from saturation, the multilayer gradually unsaturates. When H_{ext} matches the saturation field value H_{sat} of a given pixel, the pixel unsaturates. The pixel will choose its sense of rotation (black: top layer left; white: top layer right) according to so-called flipping rules (Fig. 1(a)). When $H_{ext} < \min(H_{sat})$, the whole SL is completely unsaturated (Fig. 1(b)).The set of first-neighbour rules governs the 'decision' of each pixel. In our model, all eight first neighbours have equal weights. To avoid creating domain walls, the pixel to decide chooses the colour of the majority (neighbour pixels still in saturation have no influence) or chooses by random if no decision can be made using the previous rule.

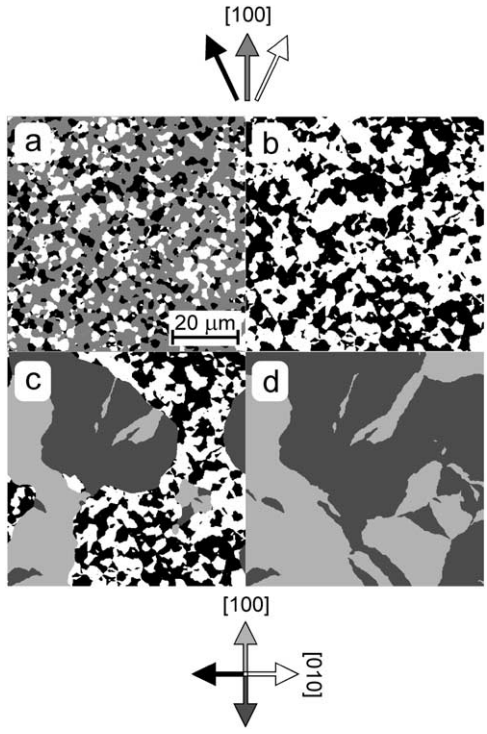

Fig. 1. Primary (a, b) and secondary (c, d) domain formation. In primary domain formation black and white pixels represent top layer rotation to the left and right, respectively, grey pixels being still in saturation. The easy axes of the fourfold anisotropy are along [1 0 0] and [0 1 0]. The sample had been saturated in the [1 0 0] direction. The grid is 500×500 pixels. The smoothing widths of the primary and secondary distributions are $w_1 = 10$ and $w_2 = 100$, respectively. In (c) and (d), the system during and after the spin flop is shown. The spin flop is induced by an increasing field along the [0 1 0] direction. Note that the secondary large domains are perpendicular to the primary small ones. Grey-scale scheme in (d): light grey pixels: top layer up, dark grey pixels: top layer down. Note that the scale was fitted to the Kerr image measured by Rührig et al. on a thick Fe/Cr trilayer [7] and not to the domains observed by SMR on a Fe/Cr multilayer of 20 periods [5].

According to this model, all domain walls are 180° walls in remanence. Indeed, assuming that the domains do not change shape having been unsaturated, but only rotate on further decrease of the field, the image is the same in remanence as in complete unsaturation (Fig. 1(b)), only the angles of the layer magnetisation directions change.

By applying an in-plane external field along the perpendicular easy axis, a bulk spin-flop transition can be induced [6]. At the transition, the pixel magnetisations rotate by $\pm 90°$. The domain nucleation of the spin flop is now governed by the distribution of the spin-flop

field, which is much broader than that of the saturation field. A pixel can choose its new direction if all pixels with lower spin-flop field have already decided. The rules are now the same as those during unsaturation, but in Fig. 1(c) the pixels may now flip from the left/right into the up/down orientation. In a simple model of the domain-wall energy, the energy penalty is proportional to the sum of the square of the relative angle of the neighbours. It can be shown that with these conditions, the secondary domain formation is independent of the primary structure and only depends on the lateral distribution of the spin-flop field. In Fig. 1(c), the small unflipped and the large flipped domains with perpendicular relative magnetisations coexist. This coexistence of perpendicularly magnetised primary and secondary domains has in fact been observed during spin flop by SMR and PNR [5]. In Fig. 1(d), the secondary domains are depicted after the spin flop has been completed.

Note that the model introduced here applies to both trilayers and multilayers as far as the two-dimensional representation holds (i.e., the coupling is strong as compared to the anisotropy energy).

To derive measurable quantities from the simulation an appropriate transformation is needed. We may choose the autocorrelation function $C(\vec{r})$ of the domain image as an indicator of the correlation length. In the Born approximation the off-specularly scattered intensity is proportional to the Fourier transform of $C(\vec{r})$.

The autocorrelation function is defined by:

$$C(\vec{r}) = \frac{\sum_{\vec{r}'}(m(\vec{r}') - \bar{m})(m(\vec{r}' + \vec{r}) - \bar{m})}{\sum_{\vec{r}'}(m(\vec{r}') - \bar{m})^2}, \quad (2)$$

where $m(\vec{r})$ is the chosen direction (colour) of the given pixel (in the PDS white: $+1$, black: -1, in the secondary domain state: light grey: $+1$, dark grey: -1), $\bar{m} = (1/L^2)\sum_{\vec{r}} m(\vec{r})$ the average of $m(\vec{r})$ and L is the width of the image in pixels. The summation goes over the complete grid.

In order to test our model, the autocorrelation function of the simulated primary domains and that of published Kerr images of Rührig et al. [7] were compared. In Fig. 2, the autocorrelation function of the model is adjusted to the autocorrelation function of the Kerr image. The agreement is quite remarkable for the mesh size of 146 nm and $w = 10$ pixels. The formal relationship between the correlation lengths of the saturation as well as spin-flop fields and the correlation length of the domains obtained as a result of the described rules has not yet been elaborated. Furthermore, due to the inapplicability of the Born approximation for the case of multiple scattering, the relation of the domain correlation length to the off-specular SMR scan shape is not a trivial task and is a subject of future study.

In summary, Monte Carlo simulations of patch-domain formation in antiferromagnetic multilayers were

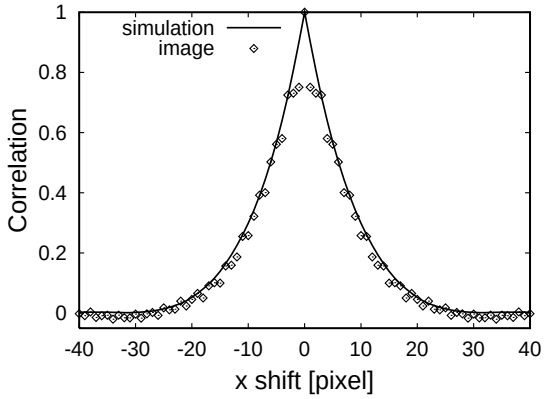

Fig. 2. The autocorrelation function (2) of the Kerr image of the AF patch-domains [7] compared with the autocorrelation function of the simulated pattern for the mesh size of 146 nm and $w_1 = 10$ pixels.

presented for the first time to our knowledge. The generated patch-domain pattern is in quantitative agreement with published Kerr-microscopic images of a Fe/Cr/Fe trilayer. The simulation describes the emergence of domains during unsaturation in accordance with observations and remarkably features the coexistence of the perpendicularly magnetised small and large domains observed by recent off-specular SMR and PNR during spin flop.

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