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# Simulation of Antiferromagnetic Domain Formation History in Magnetic Multilayers

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A Monte Carlo simulation of two-dimensional 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 domain coarsening on spin dispartial in hard direction. The simulated domain patterns are in good agreement with published Kerr microscopic images.

**1. Introduction** Antiferromagnetically (AF) coupled metallic multilayers (ML) show giant magnetoresistance (GMR) effect [1]. Recently a domain tailoring mechanism was found on an AF-coupled Fe/Cr ML with fourfold in-plane anisotropy by off-specular synchrotron Mössbauer reflectometry (SMR) and verified by polarised neutron reflectometry (PNR) [2]. Small (μm size) domains form when the external magnetic field $H_{ext}$ is decreased from the saturation to remanence. Most of these domains transform into at least one order of magnitude bigger ones (domain coarsening) on the spin flop [3–5]. A simple phenomenological model [2] and Monte Carlo simulations [6] of domain patterns were presented to reproduce the domain nucleation on 'unsaturation', i.e., on releasing the saturation magnetic field applied in an easy direction. The same algorithm with similar 'flipping rules' was applied to simulate the domain coarsening observed on spin flop [7].

In a strongly AF-coupled metallic ML of fourfold crystalline anisotropy the domain structure of the individual ferromagnetic layers is correlated through the ML stack from the substrate to the surface allowing for a two-dimensional representation of the AF domains. Easy-axis and hard-axis scenarios are qualitatively different. In our model [2] we associate the domain formation and coarsening with the effective correlation length of the saturation field $H_{sat}$ and that of the spin-flop field $H_{sf}$, respectively. Unsaturating the sample along an easy axis down to remanence leads to a single stable configuration with the magnetisations perpendicular to the field. Magnetic field and anisotropy act in the same direction. The effective correlation length of $H_{sat}$ will determine the average 'primary domain' [2] size in remanence, the anisotropy playing a minor role in the formation. On passing the spin flop in an easy-axis scenario, however, the much larger effective correlation length of the spin-flop field will dominantly determine the resulting 'secondary-domain' size and a remarkable domain coarsening effect is observed [2, 6, 7]. In a hard-direction-unsaturation scenario, however, these two phases of

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domain formation do not separate. During a coherent rotation of the domains they tend to align in one of the easy axis directions 45° relative to the field direction and, instead of a spin-flop, the system passes a 'spin dispartial' in which AF domains develop into four different orientations. Here we focus on modelling the domain formation during hard-axis unsaturation. The simulated domain patterns in remanence will be qualitatively compared with Kerr images of a Fe/Cr trilayer [8].

**2. A Model of AF-Domain Formation** We model the multilayer by a two-dimensional matrix of pixels where the 'colour' (grey-scale gradation) 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 still 'classical', i.e., consists of many columns of atoms. The different domains are formed on this grid by later explained 'first-neighbour rules'. Domains are represented as continuous regions of the same colour.

***2.1 Unsaturation domains*** The 'unsaturation' or primary AF-domain formation is governed by the distribution of $H_{\text{sat}}$ [2]. The higher the saturation field of a given pixel is, the sooner (i.e., at higher external field $H_{\text{ext}}$) the pixel unsaturates. To obtain the saturation-field distribution $H_{\text{sat}}(\mathbf{r})$, we take a grid of uncorrelated random numbers $\{U(\mathbf{r})\}$ of Gaussian distribution [9] where $\mathbf{r} = (x, y)$ is the position vector, then smooth $\{U(\mathbf{r})\}$ with an empirical function of smoothing width $w$,

$$H_{\text{sat}}(\mathbf{r}) = \sum_{|\mathbf{r}-\mathbf{r}'|<w} \left(1 - \frac{(\mathbf{r}-\mathbf{r}')^2}{w^2}\right) U(\mathbf{r}') . \tag{1}$$

Periodic boundary conditions are used throughout. We assume that $H_{\text{sat}} \gg H_{\text{sf}}$, i.e., the multilayer is strongly coupled.

Unsaturation is modelled in the following: above max $\{H_{\text{sat}}(\mathbf{r})\}$ all pixels are in saturation (represented by black and white stripes), then $H_{\text{ext}}$ is lowered. When $H_{\text{ext}}$ matches $H_{\text{sat}}(\mathbf{r})$ of the pixel at $\mathbf{r}$, the pixel unsaturates, i.e., chooses its sense of rotation (black: ML top layer *left*, white: ML top layer *right*). Creation of excess domain walls may be avoided by obeying the so-called 'flipping rules' as follows. (i) the pixel chooses the colour of the surrounding majority (all already flipped first neighbours (maximum 8) count with equal weight, pixels still in saturation having no influence) and (ii) the pixel chooses colour by random if no decision can be made according to the previous rule. At $H_{\text{ext}} = \min\{H_{\text{sat}}(\mathbf{r})\}$ the ML is completely unsaturated. The four panels of Fig. 1 are simulated snapshots of the magnetic history from saturation to remanence in a hard direction. Figures 1a to d show the 50% unsaturated state, the totally unsaturated intermediate-field state above spin dispartial, the state in 50% spin dispartial and the remanence, respectively.

The flipping rules involve only first neighbours, allowing for a fast realisation of the above algorithm. The grid is scanned for saturated pixels. When found, it is checked if all still-saturated neighbours possess a lower $H_{\text{sat}}$ value than the one found. If yes, the pixel is allowed to choose its colour according to the above flipping rules. If not, the next pixel is chosen. The scan of the grid is repeated as long as all saturated pixels flip to either black or white. Finally, the temporal evolution of the domains is reproduced and a 'movie' of the domain formation is constructed from the final state [6]. The same fast-selecting algorithm was used for the spin-flop cases [6, 7].

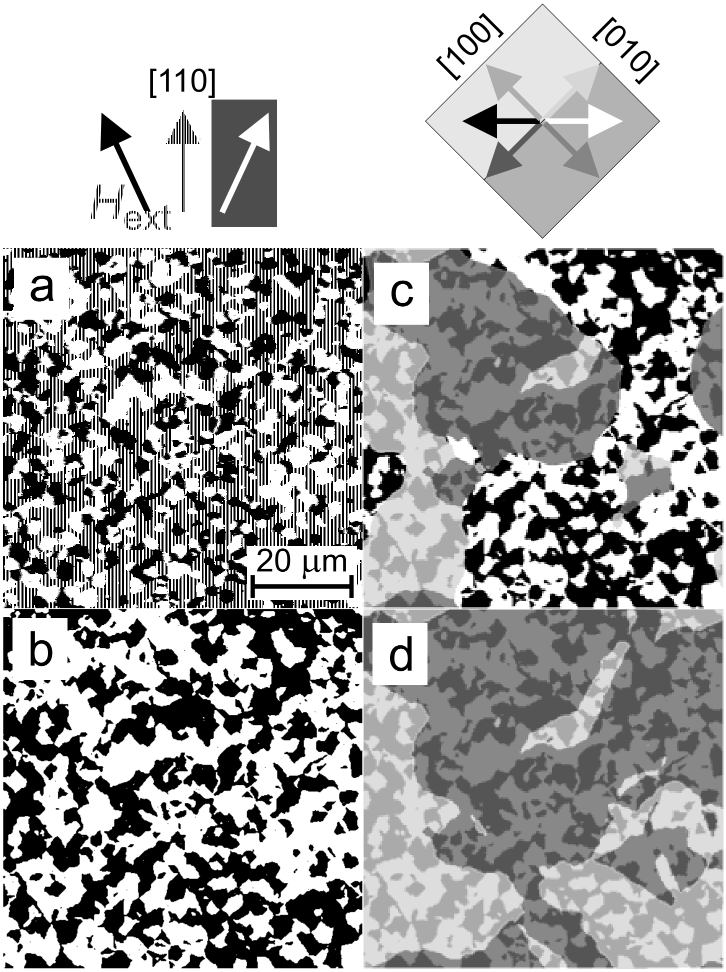


Fig. 1. Evolution of AF domain structure during unsaturation along a hard direction of the fourfold anisotropy. a) In high field, partial unsaturation, b) in intermediate field, above spin dispartial, c) following incomplete partition of domains according to the two perpendicular easy directions, d) in remanence. The grey gradation represents the direction of the top layer of a pixel according to the arrows, while the striped regions in a) are still in saturation. The easy axes of the fourfold anisotropy are directed along [100] and [010] of Fe. The grid is 500 by 500 pixels. The smoothing widths of the primary and secondary distributions are $w_1$ = 10 and $w_2$ = 100, respectively. The scale was adjusted [6] to a Kerr image measured by Rührig et al. [8] with a mesh size of 146 nm

Note that the above model applies to all compensated MLs with even number of magnetic layers (including trilayers), as far as the two-dimensional representation is valid. Provided that the bilinear coupling is strong as compared to the other energy terms, patch domains are formed close to saturation by coherent rotation, not depending either on the in-plane anisotropy or the biquadratic coupling.

***2.2 Hard-direction spin-dispartial domains*** Leaving the saturation region, the domain history starts depending on the details of the system. In the present model we assumed that $H_{sat} \gg H_{sf}$, i.e., the AF-coupling strength is the leading energy term. Thus, unsaturation along a hard magnetic axis results in close to 180° domain walls approaching a critical field $H_{sdp}$. At this field the sublayer magnetisations are directed along the hard axis perpendicular to the field, a configuration that becomes energetically unfavourable on further reducing the field. In remanence the magnetisations will lie parallel to the easy axes.

Assuming that the domains do not change shape but rotate, the domain image remains the same down to $H_{sdp}$ as it was in complete unsaturation (Fig. 1b), only the angles of the layer magnetisations change.

At the spin-dispartial field $H_{sdp}(\mathbf{r})$ the pixel magnetisations start disparting, i.e., rotating clockwise or anticlockwise (Fig. 1c). The AF domains gradually develop into four different orientations along the easy axes in remanence resulting in ±45° relative rotation from the $H_{sdp}$ state (Fig. 1d). The domain nucleation of this dispartial spin flop is now governed by the effective correlation length 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 higher spin-flop field have already decided. A left-directed pixel (e.g., top layer pointing left) can now choose between 'up-left' and 'down-left' directions. The rules are similar to the unsaturation rules, but here the energy penalty of a neighbour pixel is proportional to the square of the relative angle of the neighbours. The pixel to decide will choose the direction with the least total energy penalty. Consequently, in contrast to the easy direction spin-flop [7], in which the primary structure is 'overwritten' by the secondary domain structure, the remanent domain structure following a hard axis unsaturation 'remembers' the primary domain structure. The four types of domains are not randomly distributed, but in groups of two in order to avoid 180° domain walls as illustrated in Fig. 1d. Indeed, if a left-directed pixel has chosen to rotate left-up, a neighbouring right-directed domain will definitely rotate right-up rather than right-down since the domain-wall angle in this case will be only 90°.

To compare the simulation with already available data, the results of Rührig et al. [8] were used. The autocorrelation function of the unsaturation domain image was fitted [6] by the autocorrelation function of the digitalised image (Fig. 4b in [8]) giving the length scale in Fig. 1. A similar analysis of the hard-axis remanent state shows a good qualitative agreement, however, the image quality did not permit proper data acquisition.

**3. Conclusions** Monte Carlo simulation of patch-domain formation in antiferromagnetic multilayers was presented. The simulation describes the emergence of domains during unsaturation in high field as well as on spin dispartial in low fields. We find that releasing the external field along a hard direction results in 90° domain walls with a preferential grouping of the small domains into much larger ones the latter with net magnetisation of the top magnetic layers parallel/antiparallel to the direction of the released magnetic field. The generated pattern is in qualitative agreement with published Kerr microscopic images.

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