Supporting Information:

Quantification of Magnetic Surface and Edge States in an FeGe Nanostripe by Off-Axis Electron Holography

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February 17, 2018

Note 1: Model-based iterative magnetization reconstruction

The details of the model-based iterative magnetization reconstruction algorithm will be presented elsewhere. It is described in full in the PhD dissertation [1] of Dr. Jan Caron from the Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons and the Peter Grünberg Institute, Forschungszentrum Jülich and Aachen University, Germany. A short description of the algorithm is presented below.

According to the Aharanov-Bohm equation, the magnetic phase shift $\varphi_m(x, y)$ can
be derived from an in-plane magnetization distribution $M_{xy}$ using the expression [2, 3]

$$\varphi_m(x, y) = -\frac{\mu_0}{2\Phi_0} \int \frac{(y - y') \cdot M_x - (x - x') \cdot M_y}{(x - x')^2 + (y - y')^2} \, dx' \, dy', \quad (1)$$

where $M_x$ and $M_y$ are the $x$ and $y$ components of the magnetization, $\mu_0$ is the vacuum permeability and $\Phi_0$ is the magnetic flux quantum. This equation describes the forward problem of calculating the magnetic phase shift and can be expressed in matrix form as

$$y = F \cdot x, \quad (2)$$

where $y$ is the vectorized form of the measured magnetic phase image, $x$ is a magnetic state vector containing the retrieval target (i.e., $M_{xy}$) and $F$ is a system matrix, which is used to apply the convolutions described in Eq. 1.

The inverse problem of retrieving the in-plane magnetization distribution from a measured magnetic phase image is ill-posed, i.e., a solution for $M_{xy}$ may not exist or may not be unique. The ill-posed nature of the problem makes the direct inversion of Eq. 2 impossible, as $F$ is a rank-deficient matrix [4].

The inverse problem is solved here by applying a model-based iterative reconstruction algorithm. In a first step, the ill-posed problem is approximated by least squares minimization, which guarantees the existence of a solution. In order to en-
force uniqueness of the solution, Tikhonov regularization [5] of first order is employed to apply smoothness constraints to the reconstructed magnetization distribution. This approach is motivated by the minimization of the magnetic exchange energy of the system, which is proportional to the first spatial derivatives of the magnetization distribution. The number of retrieval targets is reduced by using a priori knowledge about the sizes and positions of the magnetized regions in the form of a two-dimensional mask. The original ill-posed problem is then replaced by the minimisation of cost function in the form

$$C(x) = \|F x - y\|^2 S_{\epsilon} - \lambda \|x\|^2 S_a. \quad (3)$$

The first Euclidean norm describes the compliance of the simulated phase image with the measurements and is weighted by a covariance matrix, which can be used to exclude parts of the phase image from the reconstruction process. The second Euclidean norm operates solely on the magnetic state vector and is weighted by a matrix, which facilitates Tikhonov regularization. Both terms are balanced against each other by using a regularization parameter. Minimization of the cost function \(C(x)\) is achieved iteratively by using a conjugate gradient algorithm [4].

Figure S4(a) describes both the forward model and the inverse problem of magnetization reconstruction from an experimentally recorded magnetic phase image. In
practice, a mask is applied to outline the boundaries of the specimen. A simulated magnetic phase image $\varphi_{mx}$ is then calculated from an initially assigned $M(x,y)$ distribution. We make use of analytical solutions for the phase shifts of simple geometrical objects, with numerical discretisation performed in real space to avoid artefacts generated by discretisation in Fourier space. This forward simulation approach is used in an iterative conjugate gradient scheme to solve the inverse problem. The flowchart shown in Fig. S4(b) describes the iterative scheme. This approach allows the exchange energy of the system to be minimized [6] by using Tikhonov regularisation of first order.

References


Figure S1: Structural characterisation of an FeGe nanostripe in the transmission electron microscope. (a) Bright-field image. (b) Electron diffraction pattern taken along an [001] zone axis. (c, d) High-resolution lattice images taken from the areas marked in (a). The scale bar in (a) is 200 nm.
Figure S2: Measurement of specimen thickness using the log-ratio method applied to energy-filtered images. (a) Thickness map calculated from energy-filtered images using log-ratio method. (b) Thickness $t$ in units of inelastic mean free path $\lambda$, extracted from the region marked in (a). (c) Schematic illustration of a thickness-wedged FeGe nanostripe with damaged layers due to focused ion beam (FIB) milling. The thickness of the damaged layers, which are magnetically inactive, is estimated to be approximately $0.2\lambda \approx 20$ nm. The dotted line marks the regions on the right of the stripe that are magnetically inactive through the entire sample thickness, as can be seen in Supporting Fig. S3. In the thickness measurement using the log-ratio method, the collection angle $\theta_C$ was $>100$ mrad. Under this condition, the inelastic mean free path $\lambda$ for cubic FeGe is calculated to be $110$ nm using the formula proposed by Iakoubovskii et al. [7].
Figure S3: Lorentz microscopy (defocused) images of the FeGe nanostripe taken at 240 K in applied magnetic fields of (a) 0, (b) 100, (c) 200 and (d) 300 mT. The images were recorded at a defocus of -400 µm. The scale bar in (d) is 200 nm.
Figure S4: Description of the model-based iterative magnetization reconstruction algorithm used in the present study. (a) Forward model and inverse problem. (b) Flow chart illustrating the iterative reconstruction of the projected in-plane magnetization from experimental magnetic phase images.
Figure S5: Histograms of the maximal in-plane magnetization measured for a single magnetic helix (in zero applied magnetic field) and a skyrmion (in an applied magnetic field of 300 mT) at 95 K. (a-c) and (d-g) show the procedure used to extract the maximal in-plane magnetization for a single helix and a single skyrmion, respectively. The blue lines marked in (b, f) show the location of the maximal in-plane magnetization. A polar transform is applied from (e) to (f). The scale bars in (a, d) are 100 nm.