2980
doi:10.1017/S1431927622011175
Microsc. Microanal. 28 (Suppl 1), 2022
© Microscopy Society of America 2022

Simulation-Trained Machine Learning Models for Lorentz Microscopy

Arthur R. C. McCray[1,2*], Amanda K. Petford-Long[1,3], and Charudatta Phatak[1]

[1.] Materials Science Division, Argonne National Laboratory, Lemont, IL, USA
[2.] Applied Physics Program, Northwestern University, Evanston, IL, USA
[3.] Department of Materials Science and Engineering, Northwestern University, Evanston, IL, USA
* Corresponding author: amccray@anl.gov

There is a rising interest in topological magnetic spin textures, such as skyrmions, for both their fundamental physical properties as well as for potential uses in next-generation spintronic devices [1]. Lorentz transmission electron microscopy (LTEM) is an appealing technique for imaging nano- and micro-scale spin textures. LTEM is compatible with a variety of *in situ* experiments and allows for simultaneous high-resolution imaging of both the magnetic structure and sample microstructure. The interpretation of LTEM images can be difficult, but one method for overcoming this is by reconstructing the electron phase shift and the integrated magnetic induction via off-axis or in-line holography techniques. This is helpful for many in-plane magnetization patterns, but for topologically nontrivial spin textures, the integrated induction can appear very different from the magnetization. A relevant example of this is the Néel skyrmion, a magnetic quasiparticle shown in Fig. 1(a). A simulated LTEM image and the integrated magnetic induction of the skyrmion are shown in Fig. 1(b) and (c), both of which appear very different than the magnetization. This discrepancy between the magnetization and reconstructed induction can lead to the erroneous interpretation of LTEM images as containing novel spin structures. Most notably, the "biskyrmion" identified with LTEM was revealed to be a canted topologically trivial bubble domain [2]. Here we present the application of PyLorentz, an open-source software suite that we have developed, for both the interpretation of topological spin structures as well as for training machine learning (ML) models that can be used to analyze experimental LTEM images.

One method for verifying complex spin structures is by comparing them to simulated data. PyLorentz allows users to define imaging conditions, such as microscope aberrations and sample tilt, and accepts as an input the magnetization output from micromagnetic simulations. It then simulates LTEM images and reconstructs the integrated magnetic induction as shown schematically in Fig. 1(d). The simulated images can be directly compared with experimental data to verify that the observed spin texture matches the known magnetization from the micromagnetic simulation. The most difficult step in the simulation is calculating the magnetic component of the electron phase shift. PyLorentz is built on a new algorithm that calculates this phase shift using a linear superposition method applicable to three-dimensional samples at any orientation [3].

Simulated image data can also be used to train ML algorithms for interpreting LTEM images. It is difficult to distinguish individual Néel skyrmions when they are in a dense lattice, especially when imaging at the high defocus necessary for working near the Curie temperature. Quantifying the size and shape of skyrmions is important as their deformation provides insight into inter-skyrmion interactions. We performed micromagnetic simulations of skyrmion lattices with varying skyrmion sizes and densities, an example of which is shown in Fig. 2(a). These magnetizations were used to create LTEM training images and ground truth labels of skyrmion sizes and locations, as shown in Fig. 2(b) and (c). A convolutional neural network trained on 5000 simulated LTEM images was applied to perform instance segmentation of the experimental image shown in Fig. 2(d). Figure 2(e) shows the output prediction

https://doi.org/10.1017/S1431927622011175 Published online by Cambridge University Press

overlaid on the input image, with the identified skyrmions transparent and the regions between skyrmions shown in red. This example demonstrates how combining LTEM image simulation with ML techniques provides new opportunities for analyzing topological spin textures in Néel skyrmion lattices and beyond [4].

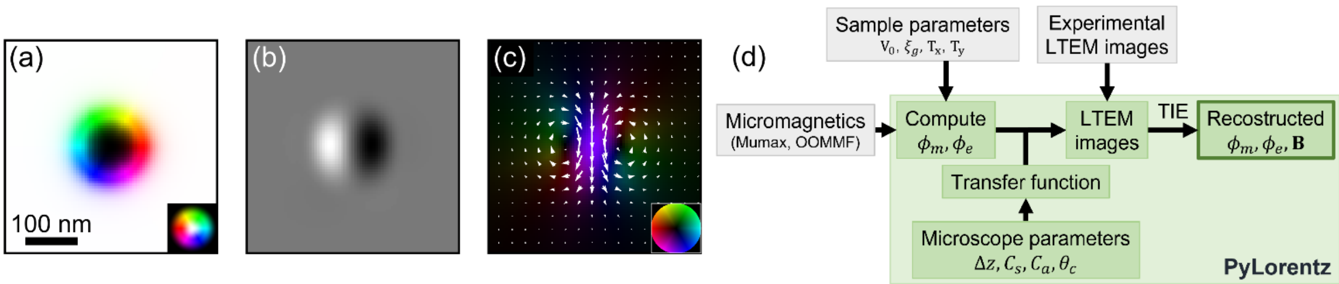

Figure 1. Néel skyrmion LTEM image simulation with PyLorentz. **(a)** Néel skyrmion magnetization, in-plane direction is depicted by the color wheel (inset), white points out of the page and black into the page. **(b)** Simulated LTEM image of the skyrmion at -1 mm defocus and 30° tilt around the *x* axis. **(c)** Integrated magnetic induction reconstructed from (b). **(d)** Flowchart showing the PyLorentz software capabilities.

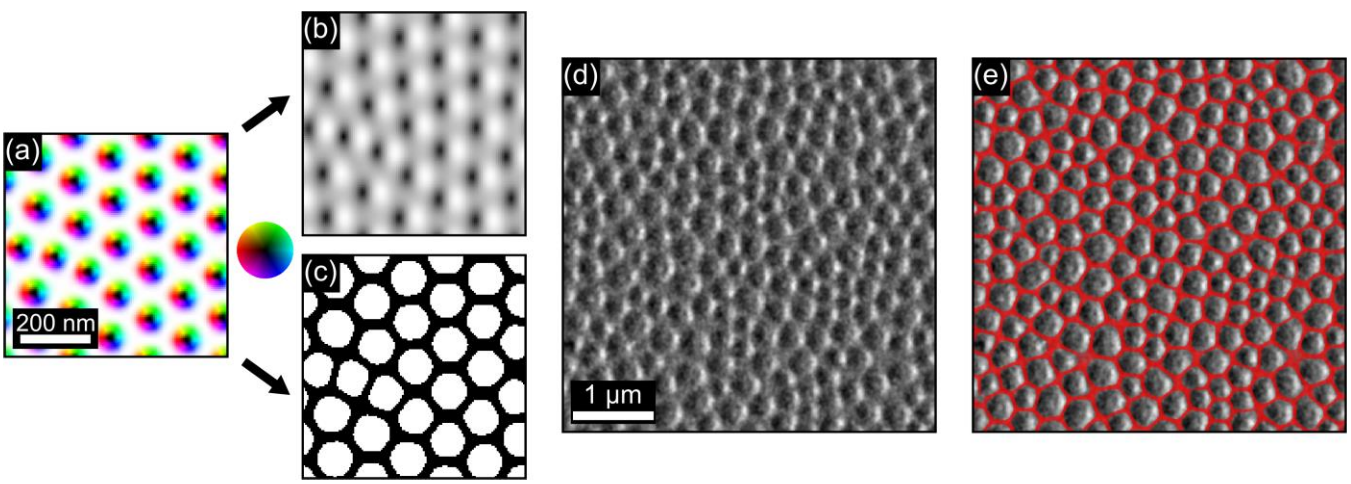

Figure 2. Machine learning applied to Néel skyrmion lattices. **(a-c)** Micromagnetic simulations of Néel skyrmion lattices (a) are used to create a training set of LTEM images (b) and ground truth labels (c). **(d)** Experimental LTEM image of a Néel skyrmion lattice in Fe_3GeTe_2. **(e)** Instance segmentation of the skyrmions performed using a CNN trained on simulated data. The CNN prediction is transparent where skyrmions are identified, red where they are not, and is shown overlaid on the input image (d).

References:

[1] Fert, A. et al. Nature Reviews Materials, **2** (2017), p. 17031. doi:10.1038/natrevmats.2017.31
[2] Loudon, J. C. et al. Advanced Materials, **31** (2019), p. 1806598. doi:10.1002/adma.201806598
[3] McCray, A. et al. Physical Review Applied, **15** (2021), p. 044025.
doi:10.1103/PhysRevApplied.15.044025

https://doi.org/10.1017/S1431927622011175 Published online by Cambridge University Press

[4] This work is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division. Use of the Center for Nanoscale Materials, an Office of Science user facility, is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

https://doi.org/10.1017/S1431927622011175 Published online by Cambridge University Press