**Original Article**

**TopoTEM: A Python Package for Quantifying and Visualizing Scanning Transmission Electron Microscopy Data of Polar Topologies**

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**Abstract**

The exotic internal structure of polar topologies in multiferroic materials offers a rich landscape for materials science research. As the spatial scale of these entities is often subatomic in nature, aberration-corrected transmission electron microscopy (TEM) is the ideal characterization technique. Software to quantify and visualize the slight shifts in atomic placement within unit cells is of paramount importance due to the now routine acquisition of images at such resolution. In the previous decade since the commercialization of aberration-corrected TEM, many research groups have written their own code to visualize these polar entities. More recently, open-access Python packages have been developed for the purpose of TEM atomic position quantification. Building on these packages, we introduce the TEMUL Toolkit: a Python package for analysis and visualization of atomic resolution images. Here, we focus specifically on the TopoTEM module of the toolkit where we show an easy to follow, streamlined version of calculating the atomic displacements relative to the surrounding lattice and thus plotting polarization. We hope this toolkit will benefit the rapidly expanding field of topology-based nano-electronic and quantum materials research, and we invite the electron microscopy community to contribute to this open-access project.

**Key words:** open source, polarization, python, STEM, topology

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**Introduction**

The advent of commercialized aberration-corrected transmission electron microscopy (TEMs) and scanning electron probe TEMs (STEMs) directly corresponds with the initial rapid increase in interest for the new field of charged ferroelectric domain wall research (Jia et al., 2008; Seidel et al., 2009; Borisevich et al., 2010). Oxide-based ferroelectric topologies were the ideal system to push the spatial resolution and showcase the use of aberration-corrected STEM technology. Concurrently, the materials science research field could now experimentally prove previously predicted exotic topological states by theoretical calculations (Catalan et al., 2011; Jia et al., 2011). Prior to the analysis of polar ferroelectric domain walls by aberration-corrected STEM, it was accepted that, unlike magnetic domain walls, ferroelectric walls were only one to two unit cells in width. However, this is in fact not the case in various ferroelectric material systems. There have been several unexpected polar and strain variations within and in the vicinity of domain walls quantified by STEM atomic displacement mapping (Das et al., 2019; Hong et al., 2021). The advancements in these two research communities have always been symbiotic, with more recently new STEM techniques such as 4DSTEM being used to map out the polarization of complex higher-order topologies such as skyrmions (Das et al., 2019) and merons (Shao et al., 2021). Additionally, ptychographic reconstructions of 4DSTEM data sets have allowed scientists to move beyond the spatial resolution possible by STEM annular dark- and bright-field detector imaging (Rothmann et al., 2020; Chen et al., 2021). In this paper, we will focus on how to extract polarization information from atomic resolution STEM data of polar ferroelectric and multiferroic topologies using post-processing software.

Initially, the few groups that had access to corrected STEMs and collaborated with ferroelectric materials thin-film growers developed code internally for the post-processing of the images. The cation displacement was quantified in the STEM images taken of domain wall topologies and thus polarization could be assigned for each unit cell. However, there has not been a unified approach to this type of STEM data analysis. Our aim as a group of TEM and ferroelectric material scientists was to make a streamlined package that could easily be used across the various communities and more specifically by non-experts in code development. We hope that this open-access software package will be developed by external users for different ferroelectric and multiferroic material systems of interest.
The TEMUL Toolkit (O’Connell et al., 2021) is a Python image and data analysis library built on Atomap (Nord et al., 2017), HyperSpy (de la Peña et al., 2021), Scikit-Image (Van der Walt et al., 2014), and other libraries. Our goal with the TopoTEM module of TEMUL Toolkit is to fill the niche of polarization mapping and general electron microscopy analysis that may not fit into the aforementioned packages, allowing researchers to contribute code—from publications or otherwise—for others to use and expand on. We also aim to bridge the gap between packages for ease-of-use, for example, combining the atom finding capabilities of Atomap with the image simulation software of PyPrismatic (Opbus, 2017; Pryor et al., 2017) and abTEM (Madsen & Susi, 2021). Currently, the TEMUL Toolkit covers a broad spectrum of analysis from extensive polarization visualization to interactive image filtering, and basic line intensity profiling to element refinement (O’Connell et al., 2021). These functions and methods are described at https://temul-toolkit.readthedocs.io and in O’Connell (2020). A guiding principle of the package is dissemination through immediate reproduction of published data analysis for a scientific and general audience. This is accomplished by in-browser Jupyter Notebooks (Kluyver et al., 2016) run within a docker (Merkel, 2014) container provided by Binder (Jupyter et al., 2018) and requires no downloads. The majority of the TEMUL Toolkit package is built upon the data structures of HyperSpy and Atomap, specifically Atomap’s sublattice class. It is therefore relatively easy for those familiar with these libraries to get started with the TEMUL Toolkit. Importing data from other languages, such as MATLAB, is also straightforward. The TEMUL Toolkit is open to any contribution, including those that lead to, or come from, published work.

The TopoTEM module of the TEMUL Toolkit has already been used in several ferroelectric topology publications, including analysis of domain walls in PbTiO₃ (Moore et al., 2020b), where the TopoTEM and signal_plotting modules were used to quantify and visualize the changing polarization. The curvature of SrRuO₃ interlayers of multi-stacked PbTiO₃ thin films was initially analyzed by the combined use of Atomap and MATLAB code in the publication by Hadjimichael et al. (2021). This was then fully adapted to Python within the TEMUL Toolkit and can now be accessed in the TopoTEM module. In both cases, the published data analysis can be verified and reproduced with a one-click Binder Jupyter Notebook running in the browser. In Moore et al. (2022), where higher order vortex topologies were analyzed, the TopoTEM module code was developed further to add in color wheels and other tools for chiral transitions visualization, as seen in the plot_polarization_vectors function. Finally, we have developed code to map out more complex unit cells distortions, and their resulting polarizations, such as in Boracite (Conroy et al., 2020). We hope this will give readers ideas to contribute code for unit cells of other polar ferroic materials systems.

In this paper, we will focus on the polarization calculation and visualization tools available within the TopoTEM module of the TEMUL Toolkit. The TopoTEM polarization module provides several functions for quick computing and visualization of atomic column polarization. The TEMUL Toolkit does not currently provide an exhaustive list of these computing methods, though contributions are welcome. First, we will describe some of the implemented methods of calculating the unit cell polarization for various materials. We will describe the extensive plot_polarization_vectors function and its various plotting parameters, as well as useful color maps available within Python. We then discuss how to average the calculated polarization over a number of squared unit cells to easily display the overall polarization in an image. We also briefly describe the lattice structure tools available within TopoTEM. Finally, examples of the code applied to existing structures are presented.

**TopoTEM Module**

Here, we describe several methods for calculating polarization (atomic column shifts), all of which output the (x, y) coordinates and (u, v) vector components. These polarization vectors can be visualized with the plot_polarization_vectors function. Figure 1 shows an example of polarization mapping workflow.

**FFT Masking and Filtering**

The fft_mapping sub-module allows one to choose the masking coordinates with choose_mask_coordinates and returns the masked fast Fourier Transform (FFT) with get_masked_ifft. This can be useful in various scenarios, from understanding the diffraction space spots and how they relate to the real space structure, to revealing domain walls and finding initial atom positions for complex unit cells or for materials where the first and second sublattice have similar z-contrast in the acquired STEM data.

**Fast Polarization Mapping**

FFT masking has traditionally been used to quickly visualize the present domain patterns in TEM and STEM images of ABO₃ polar materials such as PbTiO₃, BaTiO₃, and BiFeO₃. Such ABO₃ perovskite ferroelectrics exhibit splitting of diffraction spots in different directions related to the different polar domains due to their strain and the non-centrosymmetric property (Moore et al., 2020a). We have integrated this into the workflow of the TopoTEM module, allowing users access to numerous data processing methods for calculating polarization from STEM images in one package. Additionally, we have developed the get_masked_ifft function, which enables users to quickly monitor changes in polar topologies and associated domains for in situ experiments and thus easily produce videos of such changes in STEM image series.

Another advantage of using this masking technique is that it can help find initial sublattice atom positions for complex unit cells or less than ideal real experimental TEM/STEM data. As shown in Figure 1, FFT masking can be used as an additional step to ease the next vital and computationally heavy step of

![Fig. 1. Example analysis workflow for calculating and plotting polarization vectors from atomic resolution images. The packages given in parentheses for each step are not exhaustive. Additionally, data output from other codes, e.g., MATLAB can be input to the final plotting step.](Image)
“Find and Refine Atom Positions” using Atomap, and thus decrease the time spent finding correct atom positions. Figure 2 displays the steps required to achieve clean initial atom coordinate finding. Figures 2a–2c show the result of using the raw image for initial atom coordinate finding. In Figure 2c, it is clear that in several places, the atom coordinates are incorrectly positioned or completely missing. Figures 2d–2f shows the process of FFT masking. In Figure 2d several locations on the raw FFT are chosen using the choose_mask_coordinates function. These positions are then input to the get_masked_ifft function which outputs a filtered image. By applying the same algorithm as in Figure 2c, the overlaid atom coordinates are much improved, as shown on the FFT filtered image in Figure 2e. These are shown overlaid in Figure 2f for comparison with Figure 2c. These steps use the aforementioned functions and are found in the “Masked FFT and iFFT” section of the TEMUL Toolkit’s documentation guide.

**Find and Refine Atomic Positions**

**Plot and Visualization of Subatomic Displacements**

As summarized in Figures 1 and 2 above, the atomic coordinates of all sublattices are located and refined during the initial atomic coordinate finding routine using Atomap (or another external program). This step is followed by calculation and plotting of polarization vectors. This process has been applied to two simulation and one experimental structure in Figure 3. Example sublattices are shown in Figures 3a–3c, with red and blue markers in Figures 3a–3c indicating the first (positive) and second (negative) ionic sublattice of their structures, respectively. Figures 3d–3f displays the resulting calculated polarization vectors of each structure from Figures 3a–3c, respectively. The methods for calculating these polarization vectors are described in the following paragraph for the three example structures in Figures 3a–3c.

For classic perovskite ABO₃ polarization, Atomap provides the get_polarization_from_second_sublattice function (described at https://atomap.org). Figure 3a shows this function in use for a standard atomic structure, such as PbTiO₃. The yellow vectors in Figure 3d are plotted using the plot_polarization_vectors function. In this structure, they represent the reverse displacement of the second sublattice atomic columns (blue) relative to the center of the surrounding four first sublattice atomic columns (red) (Moore et al., 2020).

For structures that vary from the ABO₃ [001] cubic projection, the get_polarization_from_second_sublattice function cannot be used to calculate polarization. The example image in Figure 3b represents one such simulated structure, wherein the polarizable atomic columns in the blue second sublattice are not located in the center of the bright columns of red first sublattice, as in Figure 3a. The initial and final coordinates of a sublattice of atomic columns can be used within TopoTEM’s find_polarization_vectors function, which calculates the u and v components of the vector. Therefore, the initial (ideal) coordinates and refined (actual) coordinates are input to the find_polarization_vectors function to calculate the polarization. The resulting polarization vectors are displayed in Figure 3e using the plot_polarization_vectors function.

Another example of a non-ABO₃ structure ferroelectric polar material is Cu₃B₂O₇Cl (Cu, Cl based boracite) (McQuaid et al., 2017). This is an example of a polar material experimentally imaged by atomic resolution STEM for the first time, where initially we had to develop code to quantify and visualize the subatomic displacements within the TopoTEM module, as shown in Conroy et al. (2020) and in Figures 3c and 3f.

For each of the three methods from Figures 3a–3c, the resulting (x, y) coordinates and (u, v) components are output.
polarization vectors can be input and plotted with the `plot_polarization_vectors` function. Figure 3d shows the resulting polarization vector due to the cation displacement of PbTiO$_3$ previously established in literature (Shirane et al., 1970; Yadav et al., 2016). Figures 3e and 3f plots the direction and magnitude of the atomic displacement shift from the ideal structure in Figures 3b and 3c, respectively.

For some material systems the type of polarization is uniaxial and thus in theory the polarization can only be along one direction (e.g. no chirality). This is the case for structures such as uniaxial LiNbO$_3$ (Lee et al., 2010). To calculate the polarization in these materials, one uses the TopoTEM’s `atom_deviation_from_straight_line_fit` function, adapted from Gonnissen et al. (2016). Figure 4a displays the atom plane directions via the `plot_planes` sublattice method. The kink in the atom planes present in the center of Figure 4a indicates a domain wall topology. As described by Gonnissen et al., n atomic columns along the atom plane are fit to a straight line. This is repeated for the n atomic columns starting at the end of the atom plane (Gonnissen et al., 2016). The slope of the second fit is set equal to the slope of the first fit, while the y-intercept can vary. The line parallel and halfway between these two fittings is used as the line from which the \( u \) and \( v \) vector components are calculated from each atomic column. The direction of the plane of atoms, the order of fitting, as well as the number of atomic columns to use in the fitting of each plane of atoms, can be varied within the `atom_deviation_from_straight_line_fit` function. The resulting calculated polarization vectors are then visualized with the `plot_polarization_vectors` function, as shown in Figure 4b.

**Plot Polarization Vectors**

**Visualizing the Polarization**

To display the calculated polarization vectors, we use the flexible `plot_polarization_vectors` function. This function is built on the popular Matplotlib Python library (Hunter, 2007). It can be used to visualize calculated polarization in several different styles by using the parameter `plot_style`. The `plot_style` parameter currently has five options to choose from: standard vector arrows, color mapping, contour mapping, and two different color wheel displays. Each of these is displayed in Figure 5. To display the polarization vector arrows in a single color, "vector" is input for the `plot_style` parameter as shown in Figure 5a. Figure 5b displays the "colormap" option, and highlights the relative size of the vector magnitudes. Figure 5c shows the "contour" option for `plot_style`. Here, the contour colors represent the polarization angle and are partly transparent to show the underlying atomic structure for reference. One may notice that the bottom half of Figure 5c is a single color, whereas it is represented by two colors in Figures 5d-5e. This is due to the categorical cyclic color map used i.e., the green region only includes angles between 45° and 90°. The "colorwheel" option presented in Figure 5d is useful for showing the polarization vector angles at a glance. The
“polar_colorwheel” option in Figure 5e communicates the relative vector magnitude as well as the vector angle. Additionally, this allows users to use the same color scheme as the STEM differential phase contrast (DPC) color wheel plots used in commercial microscopy software such as Thermo Scientific Velox™ and JEOL 4DCanvas™.

Apart from the plot_style parameter options described above, the plot_polarization_vectors function has many parameters for modifying the plot. The polarization data may be displayed with or without the background image, as in Figures 5a and 5d, respectively. Figure 5b shows the “colormap” plot_style with a perceptually uniform color map indicating the scaled magnitudes of the vectors. The angle of the polarization vectors - which is often useful for visualizing domains – is shown with the “colorwheel” plot_style, as displayed in Figure 5c. An example of the “contour” plot_style overlaid on the image is shown in Figure 5c, with the vector angle represented by the contour map. The remove_vectors parameter was used in this case to remove the vectors from the image. For the “colormap” and “contour” plot_style mapping, the vector_rep parameter is used to display either the magnitude or the angle of the polarization vectors, as presented in Figures 5b and 5d, respectively. Setting all vectors to the same length is done by using the unit_vector parameter.

Utilizing suitable color maps allows for clear presentation of polarization in an image. Color maps are an essential part of the plot_polarization_vectors function. For example, in Figure 6 the color map is used to clearly show the upward and downward polarization as red and blue, respectively. This is much clearer than the yellow vector arrows as previously used in Figure 4b for the same material and domain wall topology. Using color maps can remove distracting information in an image and allow the user or reader to focus on the polarization trends. The color maps used in each figure in this article are either taken from the Matplotlib package’s perceptually uniform color maps or the color maps made available by the Colorcet package (which are also available through Matplotlib).

### Averaging Polarization

Atomic resolution polarization of a structure can be averaged into regions defined by a unit area using the get_average_polarization_in_regions function. The get_divide_into function is used to...
calculate a reasonable area for averaging, i.e. it will output the division needed for the desired unit cell averaging. The get_average_polarization_in_regions function’s (x, y, u, v) output can then be input to plot_polarization_vectors as described previously. Example polarization vectors averaged over 2 × 2 and 4 × 4 unit cells are shown in Figures 6b and 6c, respectively.

This function is especially useful for large images with many thousands or tens of thousands of unit cells. It allows for clear understanding of the overall polarization in the image at a glance. In future, we hope that such an analysis routine could be used during acquisition (integrated into TEM vendor software) to quickly find interesting regions or domain walls in a specimen. An example of the visualization and averaging of polarization from an experimental STEM dataset to visualize a DW topology is shown in Figure 7.

This also confirms that the plot_polarization_vectors function and in general the TopoTEM data processing module is functionally robust to distinguish between the unit cell distortions of two different polar phases of the same material system (boracite in this case) from experimental STEM data. One can see clearly the difference between the polarization plots of orthorhombic Cu–Cl boracite in Figure 3f (Conroy et al., 2020) and trigonal Fe, Mg–Cl boracite in Dowty & Clark, 1972 in Figures 7b and 7c. Additionally, using the get_average_polarization_in_regions function (Fig. 7d) allows one to visualize the polarization direction much more clearly compared to the non-averaged polarization plotting in this large field of view and complicated unit cell material.

Strain/Unit Cell Distortion

Analysing Lattice Structure

Strain engineering of ferroic materials can be used to form ferroelastic topologies and even induce ferroelectricity in nominally non-ferroelectric materials (Choi et al., 2004; Haeni et al., 2004; Schlom et al., 2007). Several research groups have shown that with precise nanoscale control of the induced strain and electrostatic boundaries conditions, non-trivial polar topologies can be created (Tang et al., 2015; Yadav et al., 2016; Zubko et al., 2016; Wang et al., 2020; Li et al., 2022). In addition to mapping out the cation and anion displacements within the unit cell, quantifying the unit cell distortion and the trends across topologies is vital to relate polarization vector with strain.

The TopoTEM module includes tools for the analysis of lattice structure such as strain, curvature, atom plane angles, and c/a ratio of unit cells. In Moore et al. (2020b) for STEM imaging of polar PbTiO3 domain wall junctions using the get_strain_map, rotation_of_atom_planes, and ratio_of_lattice_spacings functions were used to quantify and visualize the strain, atom plane angles, and c/a ratios within the field of view. Example outputs from each of these functions are shown in Figure 8 and more information on the PbTiO3 domain wall junctions can be found in Moore et al. (2020b).

The ratio_of_lattice_spacings function has also been used to calculate the shearing of unit cells in STEM imaging. For materials with such a small unit cell distortion due to structural shearing as for ferroelastic ferroelectric boracites (Zimmermann et al., 1970; McQuaid et al., 2017), strain mapping using geometric phase analysis algorithm (Hytch et al., 1998; Strain++) from STEM data is not possible. Thus, the ratio_of_lattice_spacings function provides a method to quickly check for strain coupled polar topologies present in materials, when diffraction techniques such as 4DSTEM are not possible or available. When viewing orthorhombic boracites in the [100] projection there are four in-plane and two out-of-plane domains that can be imaged. In Figure 9 the unit cell shearing and thus polarization in-plane (xy) and out-of-plane (orthogonal to xy, along the beam axis) is measured across a domain wall. The atom to atom distance is aggregated (grouped) in 10 nm thick y axis slices and averaged to display the data in Figure 9d. From left to right, the grouped mean increases and decreases by the same amount for zone 2 and zone 3, respectively. In the left, in-plane, domain there is a difference of ~15 pm between the zone 2 and 3 distortion. Moving toward the right, the grouped mean of zone 3 decreases by ~2 pm while the grouped mean of zone 2 increases by the same amount. This change in grouped mean indicates the location of the domain wall as ~15–30 nm along the x-axis. The in-plane/out-of-plane DW is inclined through the lamella, 45° to the viewing direction. So the transition from 15–30 nm reflects...
the gradual transition of the DW i.e., 0–15 nm (in-plane domain), 15–30 nm (mixed domain), and 30–80 nm (out-of-plane domain). The ~11 pm separation is therefore the unit cell distortion due to the ferroelastic primary order parameter in Cu-Cl boracite, because the domain is polarized out-of-plane. It is important to note that the thickness of the sample lamella and any zone-axis mis-tilt will affect the measured thickness of DWs that are inclined in nature to the zone-axis. Thus caution must be taken when utilizing STEM atomic displacement mapping to quantify topology thickness or inter-phases.

Curvature strain engineering research of thin-film ferroic oxides has produced several interesting polar topologies and phases results as shown recently by Ji et al. (2019) and Peng et al. (2020). A tool for calculating and visualizing curvature in SrRuO₃ and PbTiO₃ thin films was adapted from MATLAB code used in Hadjimichael et al. (2021) and is now accessible in the calculate_atom_plane_curvature function. An example use of this code on the data from Hadjimichael et al. is displayed in Figure 10.

**Conclusion**

The TopoTEM software module allows users to easily compute and visualize polarization in atomic resolution STEM images all in one package. By building on the HyperSpy and Atomap packages, among others, we have created a streamlined workflow to detect polar topologies in traditional ferroelectric materials such as PbTiO₃.
as PbTiO₃, LiNbO₃, and materials with more complex unit cells and atomic displacements such as boracites and aurivillius phases. The get_average_polarization_in_regions method extends this plotting by providing an easy method for computing the average polarization in large areas, and therefore the user can quickly identify polar regions of interest and polarization pattern trends within scans. ToPOTEM also includes several lattice structure tools allowing one to directly correlate polarization and strain per unit cell. All of the above functionality has been applied to ideal STEM simulations and more complex structures of experimentally collected STEM data. We will continue to develop this open-access package and will find widespread application in both the polar materials community and the atomic resolution STEM community at large.

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Fig. 10. (a) STEM ADF image of PbTiO₃–SrRuO₃ PbTiO₃ interfaces (b) atomic position overlaid on image (a), and (c) quantified curvature map of the SrRuO₃ layer.

Scale bar is 4 nm.
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