Multi-Pass Preprocessing for Robust Hysteresis Loop Fitting in Ferroelectric Materials

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Introduction

Hysteresis loops are experimental signatures representing the characteristics of ferroelectric materials [1]. Consequently, extracting useful features from them is crucial in describing the ferroelectric properties. However, the functional fit for hysteresis loops has difficulties in high-dimensionality of the function [2]. In this study, we aim to improve the hysteresis loop fitting of 2500 local ferroelectric hysteresis loops recorded by piezoresponse force microscopy (PFM) on a thin-film of $PbTiO_3$ at 2 μm x 2 μm over a 50 x 50 grid [3]. We fit all hysteresis loops with a physics-based nonlinear hysteresis model to characterize the properties of the associated ferroelectric materials such as polarization strength (amplitude) and coercive voltage. We obtain accurate parameter estimates by using a combination of signal preprocessing methods along with domain-aware multi-start optimization methods to ensure optimal convergence despite the presence of many coupled parameters and disparate behaviours observed among the different domains associated with those same hysteresis loops.

Methodology and Result

In the experimental hysteresis loops, there are noises and spikes to a various degree. Therefore, appropriate preprocessing is necessary before performing functional fit. As illustrated in **Figure 1**, we compare raw hysteresis loops with two preprocessing methods. The first (original) method uses absolute deviation to detect and remove spikes. However, its effectiveness is not sufficient. Thus, we propose a combined preprocessing method by adding median filter and Savitzky-Golay filter.

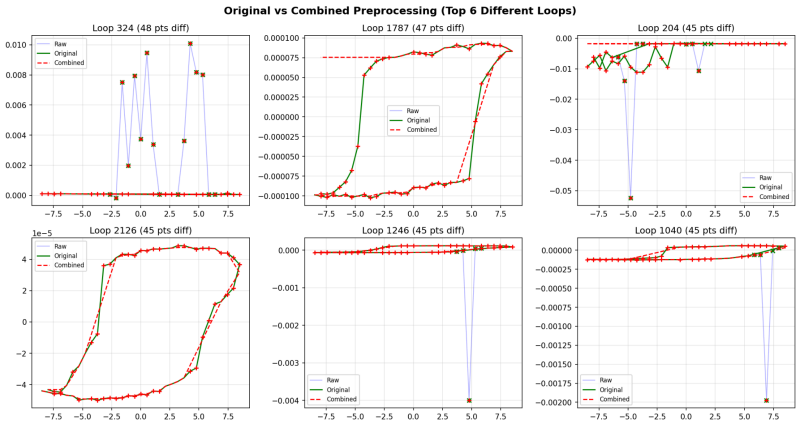

Figure 1: Hysteresis loop examples between no preprocessing (Raw), deviation-based (Original), and proposed (Combined) method

When performing functional fitting with a high parameter space, a good parameter initiation is significant for a desirable optimization result. We first employed a multi-start optimization using least square method and increasing *d* values for each optimization loop (Original). However, we observed that hysteresis loops can be further visually and numerically grouped into 3 domains

(Reversed, Normal, and Unusual) by using a classification logic based on coercive voltage signs within the loops. Hence, we proposed an improved domain-aware method of functional fitting. The result shows 4.4% reduced RMSE, indicating a slight improvement as shown in **Figure 2**. Furthermore, when mapping the domain type and result on the scan area in **Figure 3**, we found that the upper-right quadrant shows more domain mixing and unusual behavior, associating with relatively higher fit RMSE as a result.

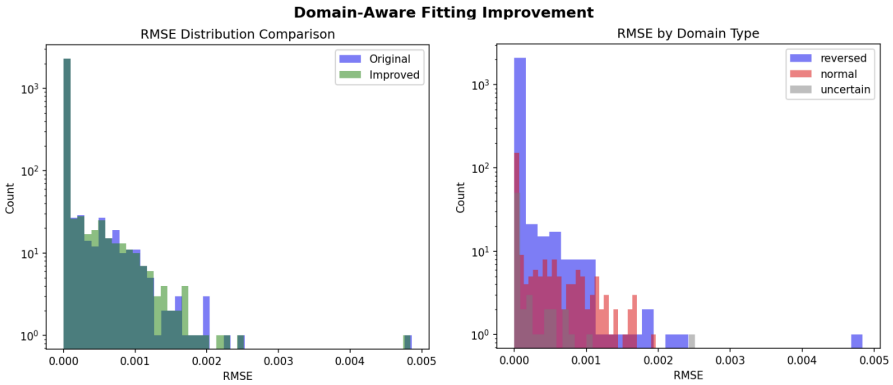

Figure 2: Fit RMSE comparison between Original and Improved method (left). RMSE distribution of Improved method based on domain type (right)

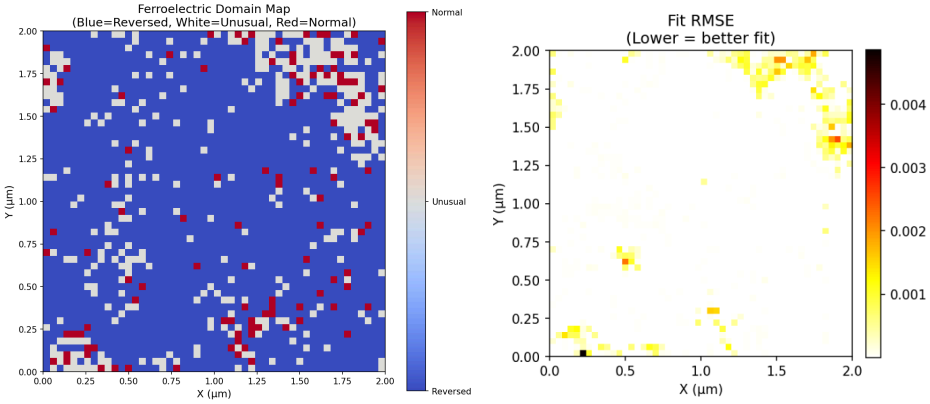

Figure 3: Simplified ferroelectric domain map based on coercive voltage signs (left). Spatial analysis of fit RMSE across the 2μm × 2μm scan area (right).

References

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