The Moiré Effect in the Scanning Transmission Electron Microscope: High Precision Structural Analysis Over Large Fields of View

A.B. Naden[1*], K.J. O'Shea[2], I. Vrejoiu[3], A. Herpers[4], R. Dittmann[4] and D.A. MacLaren[2,]
[1]School of Mathematics and Physics, Queen's University Belfast, Belfast, BT7 1NN, UK
[2]SUPA, School of Physics and Astronomy, University of Glasgow, Glasgow, G12 8QQ, UK
[3]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany
[4]Research Center Jülich, Peter Grünberg Institute, Electronic Materials (PGI-7),
52425 Jülich, Germany
*A.B. Naden: a.naden@qub.ac.uk

The properties of ferroelectric oxides are intrinsically linked to their atomic scale structure. For nanoscale structural analysis, scanning transmission electron microscopy (STEM) is a particularly versatile tool. Key advantages are the spatial resolution afforded and the variety of operating modes available. However, significant challenges remain in combining high precision with large fields of view making it time consuming to assess films with strain relaxation over large length scales or with very low dislocation densities. To this end, the moiré effect in STEM is a particularly attractive technique. Undersampling of atomic columns within a crystalline specimens leads to interference between the STEM scan pattern and the atomic lattice, producing moiré fringes over fields of view of several hundreds of nanometres. The separation and angle of these fringes are highly sensitive to variations in crystallographic spacing and angle allowing for quantification and identification of defects over these large fields of view.

Here we employ STEM moiré to characterise epitaxial perovskite systems based on $BiFeO_3$ (BFO) and $Pr_{1-x}Ca_xMnO_3$ (PCMO). We summarize a mathematical model characterizing moiré fringe formation and link it to highly accurate analysis procedures which will prove invaluable for the optimized acquisition of future datasets. We discuss the impact of large degrees of strain on the quantification of STEM moiré fringe patterns, quantify strain and identify dislocations within these crystalline materials over large fields of view up to ~ 200 nm with high precision. In BFO we identify strain relaxation over 50 nm and an estimated dislocation density of 1.6×10^{-2} nm^{-1}. We further characterize crystallographic rotation and relaxation of a PCMO lattice about large structural defects. Such assessment of crystallographic strain and defects is crucial for developing structure-function relations of functional oxides in general since their properties are inherently linked to these structural aspects. This work represents a tangible advancement in understanding this attractive approach which can be readily applied to low dose studies of damage sensitive crystalline materials.