Heterogeneous grain-scale response in ferroic polycrystals under electric field

Understanding coupling of ferroic properties over grain boundaries and within clusters of grains in polycrystalline materials is hindered due to a lack of direct experimental methods to probe the behaviour of individual grains in the bulk of a material. Here, a variant of three-dimensional X-ray diffraction (3D-XRD) is used to resolve the non-180° ferroelectric domain switching strain components of 191 grains from the bulk of a polycrystalline electro-ceramic that has undergone an electric-field-induced phase transformation. It is found that while the orientation of a given grain relative to the field direction has a significant influence on the phase and resultant domain texture, there are large deviations from the average behaviour at the grain scale. It is suggested that these deviations arise from local strain and electric field neighbourhoods being highly heterogeneous within the bulk polycrystal. Additionally, the minimisation of electrostatic potentials at the grain boundaries due to interacting ferroelectric domains must also be considered. It is found that the local grain-scale deviations average out over approximately 10–20 grains. These results provide unique insight into the grain-scale interactions of ferroic materials and will be of value for future efforts to comprehensively model these and related materials at that length-scale.

General information
Publication status: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of New South Wales, European Synchrotron Radiation Facility, Ulsan National Institute of Science and Technology
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Number of pages: 7
Publication date: 2016
Peer-reviewed: Yes

Publication information
Journal: Scientific Reports
Volume: 6
Article number: 22820
ISSN (Print): 2045-2322
Ratings:
   BFI (2016): BFI-level 1
   Scopus rating (2016): CiteScore 4.63 SJR 1.692 SNIP 1.364
Web of Science (2016): Impact factor 4.259
Web of Science (2016): Indexed yes
Original language: English
Electronic versions:
   16_BNKT_srep22820.pdf

Bibliographical note
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Source: PublicationPreSubmission
Source ID: 122160556
Research output: Contribution to journal › Journal article – Annual report year: 2016 › Research › peer-review