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Room temperature metastable monoclinic phase in $BaTiO_3$ crystals TOM LUMMEN, JIANJUN WANG, Pennsylvania State University, University Park, Pennsylvania 16802, USA, MARTIN HOLT, Center for Nanoscale Materials, Argonne National Laboratory, Argonne, Illinois 60439, USA, AMIT KUMAR, EFTIHIA VLAHOS, SAVA DENEV, LONG-QING CHEN, VENKATRAMAN GOPALAN, Pennsylvania State University, University Park, Pennsylvania 16802, USA — Low-symmetry monoclinic phases in ferroelectric materials are of considerable interest, due to their associated enhanced electromechanical coupling. Such phases have been found in Pb-based perovskite solid solutions such as lead zirconate titanate (PZT), where they form structural bridges between the rhombohedral and tetragonal ground states in compositional space. In this work, we directly image such a monoclinic phase in $BaTiO_3$ crystals at room-temperature, using optical second harmonic generation, Raman, and X-ray microscopic imaging techniques. Phase-field modeling indicates that ferroelectric domain microstructures in $BaTiO_3$ induce local inhomogeneous stresses in the crystals, which can effectively trap the transient intermediate monoclinic structure that occurs across the thermal orthorhombic-tetragonal phase boundary. The induced metastable monoclinic domains are ferroelectrically soft, being easily moved by electric fields as low as 0.5 kV cm^{-1}. Stabilizing such intermediate low-symmetry phases could very well lead to Pb-free materials with enhanced piezoelectric properties.

Tom Lummen
Pennsylvania State University, University Park, Pennsylvania 16802, USA

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