

Thermal Conductivity and Phonon Scattering Mechanisms in Ferroelectric Thin Films

Jon F. Ihlefeld,¹ Brian M. Foley,² Brian Donovan² Margeaux Wallace,³ Douglas Medlin,⁴ David Scrymgeour,¹ Linghan Ye,⁵ Bryan D. Huey,⁵ Bonnie B. McKenzie,¹ Brady J. Gibbons,⁶ D.G. Schlom,⁷ Susan Trolier-McKinstry,³ and Patrick E. Hopkins²

¹Sandia National Laboratories, Albuquerque, New Mexico/USA

²Department of Mechanical and Aerospace Engineering, University of Virginia, Charlottesville, Virginia/USA

³Department of Materials Science and Engineering, The Pennsylvania State University, University Park, Pennsylvania/USA

⁴Sandia National Laboratories, Livermore, California/USA

⁵Institute of Materials Science, University of Connecticut, Storrs, Connecticut/USA

⁶Materials Science, School of Mechanical, Industrial, and Manufacturing Engineering, Corvallis, Oregon/USA

⁷Department of Materials Science and Engineering, Cornell University, Ithaca, New York/USA

Email: jihlefe@sandia.gov

In this presentation we explore the effects of composition, phase, and morphology on the thermal conductivity of ferroelectric thin films. Thermal conduction properties in epitaxial and polycrystalline ferroelectric films comprising compositions based on BiFeO_3 , $\text{Sr}_2\text{Nb}_2\text{O}_7$, and the PZT family will be presented. It will be shown that interfaces ranging from highly disordered grain boundaries to completely coherent domain and weakly bound lattice boundaries can affect the thermal conduction through these materials. Domain boundaries, in particular, will be shown to significantly decrease thermal transport through the film thickness. Additionally, compositional dependencies on thermal conduction in PZT films are observed. The composition-dependent trends can be well described by considering the scale of the finest phonon scattering features superimposed on the trends expected from alloy scattering. This presentation represents one of the first studies of the compositional and morphology dependence of thermal conductivity in ferroelectric thin films. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.