# Thermal Conductivity of Lead Zirconate Titanate Across the Phase Diagram

B. M. Foley,[1,*] E. A. Paisley,[2] J. F. Ihlefeld[2] and P. E. Hopkins[1]
[1]Mechanical & Aerospace Engineering, University of Virginia, Charlottesville, VA, USA
[2]Sandia National Laboratories, Albuquerque, NM, USA
[*]Brian Foley: brian.m.foley@gmail.com

Lead zirconate titanate ($PbZr_{1-x}Ti_xO_3$, PZT) is an important and versatile solid-solution material system. Since its discovery in the early 1950s as an alternative to barium titanate for ceramic filters, PZT has been and continues to be a critical component in the development of many different technologies, including capacitors, electro-optic shutters, ultrasonic transducers, micro electro-mechanical systems (MEMS), and ferroelectric random access memory (FeRAM). While the past decade has seen an increasing amount of research into lead-free piezoceramic alternatives, the reality is that PZT remains the material of choice within the $20 billion piezoactuator market due to its stability, scalability and cost. [1] Despite its widespread use, knowledge of the thermal conductivity dependence on composition and microstructure is limited for PZT. Thermal conductivity can have a significant effect on the performance of a device, both in the short term as it pertains to things like sensitivity, loss tangent and operational stability, but also in the long term concerning the reliability and degradation of the device over time.

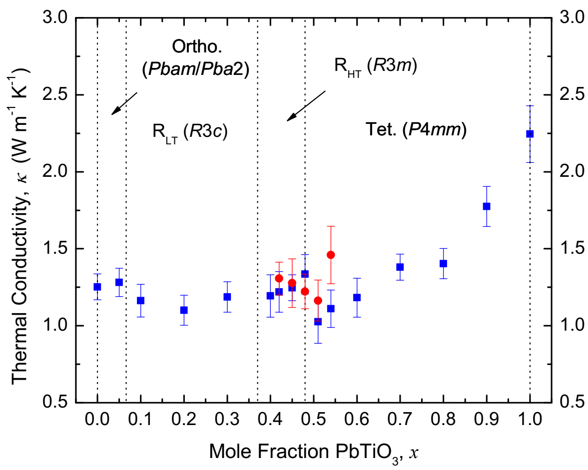


**Figure 1: Thermal conductivity of PZT thin films with various solid-solution compositions, *x*, fabricated with pyrolysis temperatures of 350°C (blue squares) and 400°C (red circles). The dashed vertical lines denote the locations of the phase boundaries in the PZT material system at 20°C.**

In this presentation, we examine the thermal conductivity of randomly oriented polycrystalline PZT thin films with compositions ranging over the entire phase diagram ($0 \leq x \leq 1$). The PZT thin films were deposited on platinized silicon substrates through chemical solution deposition (CSD), which is a commonly used means to prepare device quality PZT films. Using time-domain thermoreflectance (TDTR), we measure the thermal conductivities of PZT thin films of varying solid-solution composition, $x$. The thermal conductivity of both thin film and bulk PZT are found to vary by a considerable margin as a function of composition driven by the large difference in the thermal conductivities of the constituent materials, $PbZrO_3$ and $PbTiO_3$. Additionally, we observe a discontinuity in the thermal conductivity in the vicinity of the morphotropic phase boundary (MPB, $x = 0.48$) where there is a 20-25% decrease in the thermal conductivity in our thin film data, as well as the literature data for bulk materials. The comparison between bulk and thin film materials highlights the sensitivity of the thermal conductivity to size effects such as film thickness and grain size in even the most disordered alloy/solid-solution materials. A model for the thermal conductivity of PZT as a function of composition is presented which enables the application of the virtual crystal approximation for alloy-type material systems for parent materials with very different temperature trends for the thermal conductivity. Given the technological importance of PZT as a functional material in devices and systems, impacting a wide array of industries, this research serves to fill the gap in knowledge regarding the thermal properties.

## References

[1] J. Rödel *et al.*, *J. Eur. Ceram. Soc.*, **35**, 1659 (2015)