Studying Thermoelectric Oxides using High-Resolution Scanning Transmission Electron Microscopy

The environmental impact of global climate change due to the combustion of fossil fuels is becoming increasingly alarming. In addition, the world's rising demand for energy is causing a dramatic escalation of social and political unrest. Finding alternative fuel resources that will reduce our current greenhouse-gas emissions and dependence on foreign crude-oil is therefore not only an environmental, but most importantly, a national-security issue. While the majority of current research on alternative energy is focused on either carbon-based fuels or wind and solar energy, approaches that are portable, minimize the environmental impact, and deliver energy continuously, such as thermo-electric power generation, have often been overlooked. Thermo-electric (TE) power applications offer a potentially cheap, pollution- and maintenance-free alternative to convert heat into electricity. This approach relies on scavenging waste heat from automotive exhausts or industrial processes, all of which generate enormous amounts of unused waste heat, and converting it to electricity via the use of TE devices. As these generators are solid-state devices with no moving parts, they are silent, reliable and scalable, making them ideal for small, distributed power generation.[1]

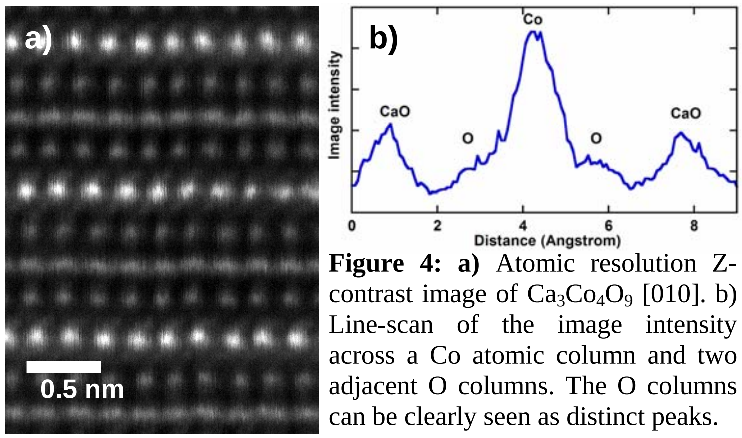

Figure 4: a) Atomic resolution Z-contrast image of $Ca_3Co_4O_9$ [010]. b) Line-scan of the image intensity across a Co atomic column and two adjacent O columns. The O columns can be clearly seen as distinct peaks.

In this research project, the PI will utilize atomic-resolution Z-contrast imaging[2-4] and electron energy-loss spectroscopy (EELS) in a scanning transmission electron microscope (STEM) of $Ca_3Co_4O_9$ (see Figure 4 and Figure 5) to develop a fundamental understanding of how changes in the atomic structure drive the exceptionally high thermoelectric Seebeck coefficient, *S*, in this class of misfit layered cobalt oxides. The PI Klie is an expert in atomic-resolution characterization of oxides, and has recently received funding (NSF MRI-R^2; $1,999,999; 3/10-2/12) for the acquisition of a state-of-the-art aberration-corrected, cold-field emission gun scanning transmission electron microscope. This instrument will enable simultaneous annular bright field and high-angle annular dark field imaging (see Figure) with 60 pm spatial and 300 meV energy resolution in the temperature regime between 20 K and 1300 K.

The REU student will be involved in the structural characterization of the thin-film materials synthesized by pulsed laser deposition. In particular, the REU student will be responsible for imaging the interface between the substrate and the $Ca_3Co_4O_9$, determining the epitaxial relationship between the substrate and the support for a larger number of different substrates (e.g. $SrTiO_3$, Al_2O_3, Si), and measuring the grain-size and texture of the thin film. The data obtained by the REU student will be crucial in correlating the thermoelectric transport properties with the film synthesis, which will lead to a number of high-impact publications, and potentially presentation at local conferences.

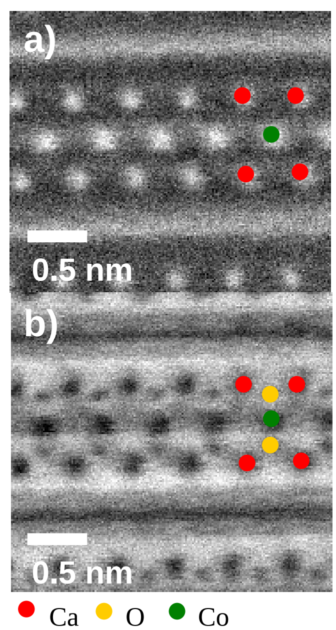

Figure 5: Atomic-resolution a) Z-contrast image and b) annular bright-field (ABF) image of $Ca_3Co_4O_9$ [110]. The Z-contrast image shows the Co and Ca columns, the ABF image also shows the O columns.

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1. Snyder, G.J. and E.S. Toberer, *Complex thermoelectric materials.* Nature Materials, 2008. **7**(2): p. 105-114.

2. Browning, N.D. and S.J. Pennycook, *Atomic resolution spectroscopy for for microanalysis of materials.* Microbeam Analysis, 1993. **2**: p. 81-89.
3. Pennycook, S.J. and D.E. Jesson, *High-Resolution Incoherent Imaging Of Crystals.* Physical Review Letters, 1990. **64**(8): p. 938-941
4. Yang, G., Q. Ramasse, and R.F. Klie, *Direct measurement of charge transfer in thermoelectric* $Ca_3Co_4O_9$*.* Physical Review B, 2008. **78**(15): p. 153109.