Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Structure and Stoichiometry in doped LLZO ($Li_7La_3Zr_2O_{12}$) MICHELLE JOHANNES, Naval Research Laboratory, NOAM BERNSTEIN, NRL, ASHFIA HUQ, Oak Ridge National Laboratory, SAIKAT MUKHOPADYAY, ORNL, JEFF WOLFENSTINE, Army Research Laboratory, JAN ALLEN, ARL, TRAVIS THOMPSEN, University of Michigan, JEFF SAKAMOTO, UMich, DEREK STEWART, HGST — LLZO has a tetragonal, Li-ordered phase with very low ionic conductivity and a cubic, Li-disordered phase with two orders of magnitude higher conductivity, relevant for solid electrolyte usage. The jump in conductivity can be correlated to dopant-induced Li vacancies that disorder the Li sublattice and cause the structural phase transition. In this work, we use extremely careful synthesis, neutron diffraction, synchrotron XRD, Raman scattering, and first principles techniques to show how both overall structure and selected local structural elements change as a function of dopant concentration. In particular, we examine how the local structure that defines the Li ion pathways changes with the lattice constant and how important microscopic quantities such as different Li site energies and hopping barriers change accordingly. Our work provides a link between the easily measurable lattice constant and extremely important but difficult to measure performance indicators such as exact Li vacancy concentration and hopping energy barriers. We hope that the "map" between structure and property provided here will speed optimization of the ionic conductivity via targeted doping strategies.

Michelle Johannes
Naval Research Laboratory

Date submitted: 12 Nov 2014 Electronic form version 1.4