

Short-range-order in $(\text{ZnSnN}_2)_{1-x}(\text{ZnO})_{2x}$ as Examined by EELS Fine Structure

Allison Mis^{*1}, Celeste Melamed¹, Geoff L Brennecke¹, Adele Tamboli², Nestor J Zaluzec³, Thomas Gage³, Jianguo Wen³

¹. Metallurgy and Materials Department, Colorado School of Mines, Golden CO, USA

². National Renewable Energy Laboratory, Golden CO, USA

³. Argonne National Laboratory, Lemont IL, USA

* Corresponding Author: amis@mines.edu

Zinc tin nitride has shown promise for optoelectronic applications, and when doped with oxygen it is expected to form a solid solution with ZnO, $(\text{ZnSnN}_2)_{1-x}(\text{ZnO})_{2x}$. Short-range order (SRO), i.e. what proportion of the anion's first nearest neighbors are zinc vs tin, has been shown to influence optical properties. The various possibilities for an anion and its first nearest neighbors are referred to as motifs. At the composition $x=0.25$, it is possible for the material to consist of only motifs that satisfy the octet rule, a phenomenon known as perfect short-range ordering (PSRO).

Previous work has correlated absorption edge onset in samples at the PSRO composition with short-range order as measured by X-ray absorption near edge structure (XANES) measurements. The samples in that study, thin films grown by RF co-sputtering, span a range of growth and annealing conditions that likely cause the variation in short-range order. However, it was not known how homogeneous the short-range ordering is due to the mm-scale sampling region of XANES.

In this work, we have carried out a variety of spatially-resolved electron energy-loss spectroscopy (EELS) measurements of the same thin-film samples, focusing on the fine structure of the O and N peaks. These measurements show variation in fine structure across samples, similarly to the XANES measurements in reference 1, but they also show variation in fine structure across sample features such as grain boundaries. Computational predictions help to correlate fine structure features with particular SRO motifs and relate the observed EELS data to the existing XANES SRO measurements. The EELS measurements will be combined with chemical mapping to show the homogeneity of anion and cation distribution in the thin film [1].

References:

[1] The authors acknowledge funding from the CoorsTek Fellowship, through the Colorado School of Mines Foundation. This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Workforce Development for Teachers and Scientists, Office of Science Graduate Student Research (SCGSR) program. The SCGSR program is administered by the Oak Ridge Institute for Science and Education for the DOE under contract number DE-SC0014664. Funding and support was also received from the Center for Nanoscale Materials and the Photon Science Directorate of Argonne National Laboratory, funded by the Office of Science, of the U.S. Department of Energy under contract number DE-AC02-06CH11357.