MS42-P09 | SPACE- AND TIME-RESOLVED ANALYSIS OF THE DECOMPOSITION OF THERMOELECTRIC MATERIALS WITH MOBILE ATOMS UNDER WORKING CONDITIONS

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Mixed ionic and electronic conductors such as Cu2-xSe [1] or Zn4Sb3 [2] have attracted much interest as thermoelectric materials, but tend to decompose under electrical currents due to electromigration of Cu or Zn. This is complicated by transitions to superionic HT phases, whose stability interval depends on the (changing) composition. This decay can be simulated in stress tests applying external currents, which were done for several materials. In addition to *ex situ* measurements, X-ray computed diffraction tomography (XRDCT) with microfocused high-energy synchrotron beams at beamline ID15A (ESRF) yields time and space resolved information under *operando* conditions. It yields 3D resolved powder diffraction data with ca. 25 µm spatial resolution, which, in principle, allow the mapping of all information that is present in diffraction patterns. Samples of Cu2-xSe were investigated *in situ*, applying various currents and temperature gradients. 3D-XRDCT reconstructions reveal the Cu migration in Cu2Se even at low temperatures even though it had only been described for the superionic phase.[1] Mapping the content of the cubic HT phase shows how it may form at both electrodes and how the boundary between ordered and disordered phases moves as a function of time. This unique access to *in situ* data of MIECs can explain the changing transport properties of a broad range of thermoelectric materials.

[1] D. R. Brown, T. Day, T. Caillat, G. J. Snyder, Mater. **42**, 2014 (2013).
[2] G. J. Snyder, M. Christensen, E. Nishibori, T. Caillat, B. B. Iversen, **3**, 458 (2004)