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Structural Order and Thermodynamic Stability of Disordered Cu_2ZnSnS_4 Alloys[1] SIN CHENG SIAH, RAFAEL JARAMILLO, Massachusetts Institute of Technology, PETE ERSLEV, GLENN TEETER, National Renewable Energy Laboratory, TONIO BUONASSISI, Massachusetts Institute of Technology — Crystalline kesterite Cu_2ZnSnS_4 (c-CZTS) thin films, of interest for photovoltaics, has a narrow window of thermodynamic stability and complex point defect chemistry. Hence, c-CZTS solar cells are thought to suffer from the effects of secondary phase segregation and further improvements in device efficiency may hinge on using kinetic stabilization to inhibit decomposition. By growing films at room temperature (T), we achieve a disordered $(CuZnSn)S_4$ alloy with an expanded solid solution window in the pseudo-ternary CuS–ZnS–SnS phase diagram that allows independent tuning of bandgap and carrier concentration. We use extended x-ray absorption fine structure to quantify short range order, and x-ray absorption near edge structure to quantify phase segregation of this new alloy. X-ray diffraction is used to elucidate the long range structural order. We study the structural evolution of the alloy as a function of annealing temperature and see continuous evolution towards c-CZTS phase that is nearly complete at 450°C. Our results inform the fabrication of conventional c-CZTS solar cells by establishing the temperature range over which thin films transform from a kinetically stabilized, metastable phase to a thermodynamically stabilized, crystalline phase.

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