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X-ray absorption spectroscopy to investigate the doping mechanism in amorphous $\mathbf{Cu_2ZnSnS_4}$ thin films[1] SIN CHENG SIAH, RUPAK CHAKRABORTY, Massachusetts Institute of Technology, PETER ERSLEV, GLENN TEETER, National Renewable Energy Laboratory, CHENJUN SUN, Argonne National Laboratory, TONIO BUONASSISI, Massachusetts Institute of Technology — Recently, Teeter *et al.* at NREL have discovered that Cu_2ZnSnS_4 thin films, of interest for photovoltaics, are amorphous (a-CZTS) when grown at room temperature and the film resistivity can be tuned over a wide range by controlling the Cu:Sn ratio. Tetrahedrally-coordinated amorphous semiconductors belong to an interesting class of compounds that are predicted to have the ability of being doped both p- and n-type. The four-fold coordination plays a critical role in unpinning the Fermi level to allow effective control over doping levels in a disordered structure. We performed extended X-ray absorption fine structure spectroscopy at the K-edges of Cu, Zn and Sn to determine the extent of structural disorder and tetrahedral coordination in a-CZTS films grown with varying Cu:Sn content. All films exhibit a high degree of structural disorder beyond the cations' first coordination shell. Both Cu and Zn atoms have high degree of tetrahedral coordination with respect to S atoms while the average coordination number of Sn decreases with increasing Sn content, indicative of either the favorable formation of sulfur vacancies around Sn atoms or the presence of Sn-related secondary phase. We combine these results with conductivity measurements to understand the relationship between the structural and electrical properties of this new material.

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