The Crystal Structure of $(Cu_xZn_{1-x})_{0.456}In_{1.084}Ge_{0.46}O_3$ (CuZIGO) Using Neutron and X-ray Diffraction

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The solid solution $(Cu_xZn_{1-x})_{0.456}In_{1.084}Ge_{0.46}O_3$ (CuZIGO) has a complex structure where zinc and copper partially occupy a site shared by indium and germanium. ZIGO, the $x = 0$ endpoint, is a potential transparent conducting oxide (TCO) with similar conductivity and transparency to In_2O_3, which, when doped with Sn^{4+}, is the most prevalent TCO. The incorporation of copper in the ZIGO structure was studied using both neutron and x-ray diffraction. Neutron diffraction is important for analyzing CuZIGO because of the negligible contrast in x-ray scattering power between copper and zinc. Using Rietveld analysis of neutron data collected at the High-Flux Isotope Reactor, copper was localized at the 16f site of tetragonal $(Cu_xZn_{1-x})_{0.456}In_{1.084}Ge_{0.46}O_3$ where $x = 0.25$ and 0.5. No copper was found in any of the three other cation sites (8e, 4a or 4b, which are occupied by indium, indium and germanium, respectively in the ZIGO compound). The lattice parameters of the solid solution $(Cu_xZn_{1-x})_{0.456}In_{1.084}Ge_{0.46}O_3$ where $x = 0.25$, 0.50, 0.75, and 1.00 were investigated with high-resolution synchrotron diffraction data collected at the Advanced Photon Source. NSF-MRSEC grant number DMR-1720139 funded this research.