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Structural Properties of Amorphous Indium-Based Oxides RABI KHANAL, JULIA MEDVEDEVA, Missouri University of Science and Technology — Amorphous transparent conducting and semiconducting oxides exhibit similar or even superior properties to those observed in their crystalline counterparts. To understand how the structural properties change upon amorphization and how chemical composition affects the local and long-range structure of the amorphous oxides, we employ first-principles molecular dynamics to generate amorphous In-X-O with X=Zn, Ga, Sn, Ge, Y, or Sc, and compare their local structure features to those obtained for amorphous and crystalline indium oxide. The results reveal that the short-range structure of the Metal-O polyhedra is generally preserved in the amorphous oxides; however, different metals (In and X) show quantitatively or qualitatively different behavior. Some of the metals retain their natural distances and/or coordination; while others allow for a highly distorted environment and thus favor "defect" formation under variable oxygen conditions. At the same time, we find that the presence of X increases both the average In-O coordination and the number of the 6-coordinated In atoms as compared to those in IO. The improved In coordination may be responsible for the observed reduction in the carrier concentration as the substitution level in In-X-O increases.

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