Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Structural and electronic properties of amorphous ternary and quaternary oxide semiconductors[1] K. NOCONA SANDERS, RABI KHANAL, JULIA E. MEDVEDEVA, Missouri University of Science and Technology — Amorphous structures of several multi-cation wide-bandgap oxides (In-Ga-Zn-O, In-Sc-O, In-Y-O, and In-La-O) were obtained via first-principles molecular dynamics liquid-quench approach using different cooling rates and different oxygen and metal compositions. A detailed comparison of the structural properties, namely, the distribution of metal-oxygen (M-O) and metal-metal (M-M) distances, bond angles, and coordination, allows us to determine how the MO polyhedra network is affected by the crystalline-to-amorphous transition. Furthermore, the role of oxygen non-stoichiometry in defect formation is investigated. Specifically, local structural defects associated with severe distortions in the metal-oxygen polyhedra, such as under-coordinated metal and oxygen atoms, or M-M bonds, appear in the electronic band structure of amorphous oxides. Both carrier-generating defects and carrier trapping/scattering defects are identified. The results help determine the optimal composition and preparation conditions (i.e., oxygen partial pressure, deposition temperature) in order to achieve the desired properties of the technologically-appealing amorphous oxide semiconductors.

[1]NSF-MRSEC

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Date submitted: 06 Nov 2015 Electronic form version 1.4