MAR16-2015-009557

Abstract for an Invited Paper
for the MAR16 Meeting of
the American Physical Society

Structure and Properties of Amorphous Transparent Conducting Oxides[1]

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Driven by technological appeal, the research area of amorphous oxide semiconductors has grown tremendously since the first demonstration of the unique properties of amorphous indium oxide more than a decade ago. Today, amorphous oxides, such as a-ITO, a-IZO, a-IGZO, or a-ZITO, exhibit the optical, electrical, thermal, and mechanical properties that are comparable or even superior to those possessed by their crystalline counterparts, pushing the latter out of the market. Large-area uniformity, low-cost low-temperature deposition, high carrier mobility, optical transparency, and mechanical flexibility make these materials appealing for next-generation thin-film electronics. Yet, the structural variations associated with crystalline-to-amorphous transition as well as their role in carrier generation and transport properties of these oxides are far from being understood. Although amorphous oxides lack grain boundaries, factors like (i) size and distribution of nanocrystalline inclusions; (ii) spatial distribution and clustering of incorporated cations in multicomponent oxides; (iii) formation of trap defects; and (iv) piezoelectric effects associated with internal strains, will contribute to electron scattering. In this work, ab-initio molecular dynamics (MD) and accurate density-functional approaches are employed to understand how the properties of amorphous ternary and quaternary oxides depend on quench rates, cation compositions, and oxygen stoichiometries. The MD results, combined with thorough experimental characterization, reveal that interplay between the local and long-range structural preferences of the constituent oxides gives rise to a complex composition-dependent structural behavior in the amorphous oxides. The proposed network models of metal-oxygen polyhedra help explain the observed intriguing electrical and optical properties in In-based oxides and suggest ways to broaden the phase space of amorphous oxide semiconductors with tunable properties.

[1]The work is supported by NSF-MRSEC program