Fundamentals of Amorphous Oxide Semiconductors

Amorphous oxide semiconductors (AOS)—ternary or quaternary oxides of post-transition metals—have attracted a lot of attention due to high carrier mobility which is an order of magnitude larger than that of amorphous silicon (a-Si:H). Unlike Si-based semiconductors, AOS exhibit optical, electrical, thermal, and mechanical properties that are comparable or even superior to those possessed by their crystalline counterparts. However, the properties of AOS are extremely sensitive to deposition conditions, oxygen stoichiometry, and metal composition, rendering the available research data inconsistent or hard to reproduce, thus, hampering further progress. Moreover, owing to the weak metal-oxygen bonding as well as many degrees of freedom in disordered materials, defects in AOS have the structural, thermal, and electronic characteristics that differ fundamentally from those in the crystalline transparent conducting oxides.

To navigate the large parameter space for AOS materials, computationally-intensive ab-initio Molecular Dynamics simulations followed by comprehensive structural analysis and accurate Density-Functional calculations, are performed for several AOS families. Integrated with systematic experimental measurements, the results provide microscopic understanding of complex relationships between the morphology, carrier generation, and electron transport across the crystalline-amorphous transition and help derive versatile design principles for next-generation transparent amorphous semiconductors with a combination of properties not achievable in Si-based architectures.

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Tuesday, January 14th, 2020
Cook Hall, Rm. 2058, 2:00-3:00 p.m.