

The Structure and Properties of Amorphous Indium Oxide

D. Bruce Buchholz¹, Qing Ma², Diego Alducin³, Arturo Ponce³, Miguel José-Yacamán³, Rabi Khanal⁴, Julia Medvedeva⁴, Robert P.H. Chang¹

¹Northwestern University Materials Research Science & Engineering Center

²DND-CAT, Northwestern Synchrotron Research Center, APS, Argonne National Laboratory

³Department of Physics and Astronomy, University of Texas at San Antonio

⁴Department of Physics, Missouri University of Science & Technology

Indium oxide thin films deposited by Pulsed Laser Deposition have local maxima in carrier mobility in the transition region between amorphous and crystalline phases. Using Molecular Dynamics Liquid Quench simulations, and validated by agreement with Extended X-ray Absorption Fine Structure measurements, a possible mechanism for this observation has been proposed. As the cooling rate in the MD simulations is decreased the amorphous structure changes from containing small isolated InO_6 clusters, to ones containing InO_6 chains, and finally to those containing large isolated InO_6 clusters. Local maxima in carrier mobility are also observed in the transition regions for more complex oxides, such as zinc-indium-tin oxide.

