Abstract Submitted
for the PSF20 Meeting of
The American Physical Society

Kinetic Monte Carlo Investigations of Metal-Oxide Atomic Layer Deposition DAVID MAGNESS, BIKASH TIMALSINA, EMILY JUSTUS, DAVID MAGNESS, Missouri State University - Dept. of Physics, Astronomy, and Materials Science, SAKIDJA RESEARCH GROUP TEAM — ATOMIC LAYER DEPOSITION (ALD) OF ULTRA-THIN METAL-OXIDES (SUCH AS ZNO OR AL2O3) AS THE CANDIDATE MATERIALS FOR ULTRA-THIN TUNNEL BARRIER LAYERS IS OF GREAT RESEARCH INTERESTS. IN THIS STUDY, WE ADOPT A 3D ON-LATTICE KINETIC MONTE CARLO (KMC) CODE DEVELOPED BY TIMO WECKMAN'S RESEARCH GROUP TO INVESTIGATE THE ROLE OF VARIOUS EXPERIMENTALLY RELEVANT FACTORS ON THE SIMULATED GROWTH OF ZNO LAYER. THE RESULTS FROM THE MODIFIED CODE INTENDED TO SIMULATE THE DEPOSITION OF AL2O3 ARE ALSO PRESENTED. ADJUSTABLE PARAMETERS INCLUDE CHAMBER PRESSURE AND TEMPERATURE, PULSE/PURGE TIMES, AS WELL AS THE STATE OF THE INITIAL SURFACE. THE ACCUMULATED DATA FROM THE CODE YIELDS INFO ON THE SIMULATED STRUCTURE, STOICHIOMETRY, MASS-GAIN, AND THE REACTION TYPES & THEIR RESPECTIVE OCCURRENCE FREQUENCY. THE RESULTS ARE THEN COMPARED TO EXPERIMENTAL RESULTS FROM LITERATURE AND PREDICTIONS FROM AN AI TRAINED ON THE SIMULATED DATA. THE SUPPORT FROM NSF (EPMD DIVISION) AWARD NO. 1809284 IS GRATEFULLY ACKNOWLEDGED.

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Date submitted: 31 Oct 2020 Electronic form version 1.4