GEC20-2020-000369
C

Abstract for an Invited Paper
for the GEC20 Meeting of
the American Physical Society

Reaction Network Analysis for Atomic Layer Deposition Processes[1]

RAYMOND ADOMAITIS, University of Maryland

Modeling the dynamics of atomic layer deposition processes is challenging because of the nonlinear behavior of these systems, their multiple and widely-ranging timescales, and by the relative lack of validated reaction kinetics information. Those data that do exist are typically derived from quantum chemical computations or experimental examinations of reaction sequences that define only a portion of the complete ALD reaction cycle. In this talk, I will describe our efforts to develop mathematical methods that address the numerical challenge of simulating dynamic ALD processes while providing a rational path to creating well-posed models of these deposition processes. Our model reduction approach is based on a two-step procedure where in the first step, the chemical species surface balance dynamic equations are factored to decouple the (nonlinear) reaction rates, eliminating redundant dynamic modes. The second phase further reduces the dynamic dimension when species relatively minor in concentration can be identified. The overall technique extracts physically significant reaction invariants and points to potential model structural problems if they exist.

[1]National Science Foundation