

Abstract Submitted  
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**Development of reactor scale model of a batch reactor for ALD processing**<sup>1</sup> EVRIM SOLMAZ, SUDHARSHANARAJ THIRUPATHIRAJ, University of Texas at Austin, SEUNG-MIN RYU, Samsung Electronics Co., Ltd., LAXMINARAYAN L. RAJA, University of Texas at Austin — We report on the development of high-fidelity computational model of a chemical vapor deposition (CVD) reactor process for silicon-based atomic-layer deposition (ALD) applications. The low-pressure reactor scale process involves flow, volume chemistry, and deposition of thin film at multiple wafer surfaces. A full 3D computational representation of the reactor is developed including the multiscale geometric fidelity of the large meter-scale reactor volume and the mm-scale interwafer gap. The fluid mechanics within the reactor are described using a continuum as well as a pure particle-based (DSMC/MCC) method. A chemistry model for the hexachlorodisilane (HCD) gas precursor and nitrogen carrier gas decomposition in the reactor is developed and implemented with both continuum and particle models. The study reports on both the physics of reactor scale phenomena to identify rate limiting steps and the uniformity of the deposition process at the wafer. In addition, computational metrics of the model such as accuracy and computational times associated with the continuum and particle approaches are discussed.

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