Three-Dimensional TCAD for Atomic Layer Processing

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The continuing progress in device miniaturization requires critical dimension control to the order of nanometers. This has led to the development of advanced processing techniques, notably atomic layer deposition (ALD) and atomic layer etching (ALE) [1]. The idealized concept behind these techniques is to split the process into a series of self-limiting half-steps, enabling monolayer control. Conceptually, this should be possible due to complete surface coverage. However, the intricacies of the real chemical processes have led to the development of several models clarifying the properties of the actual processes. ALD has been studied with respect to its fundamental surface chemistry through density functional theory and lattice kinetic Monte Carlo (KMC) simulations [2]. Although invaluable, these atomistic simulations are too computationally expensive to be directly integrated within a feature scale simulator. Alternatively, feature scale voxel-based approaches have been applied to ALD [3] and ALE [4]. They are similar in concept to the lattice KMC approach, but the atomistic representation is replaced with rectangular cells containing a material mix. This approach requires the assembly of a large list of surface reactions and it cannot be straightforwardly integrated into a typical technology computer-aided design (TCAD) workflow. Analytical models are also an active area of research, having been applied to parameter estimation in certain ALD processes [5]. Conventional TCAD tools [6] often struggle with atomic layer processes. In this presentation, we will show how surfaces and their chemistry are described in process TCAD, including possible extensions. Particular attention is placed on the role of the steady-state approximation of surface coverage and how models are introduced to the transient regime.

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