An Extended Knudsen Diffusion Model for Aspect Ratio Dependent Atomic Layer Etching

4:15pm - 4:30pm Room Regency Ballroom A-C
Tue, Jul 23 ALE2-TuA12

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Atomic layer etching (ALE) is a fundamental part of semiconductor processing as device critical dimensions must be controlled to the order of nanometers [1]. One known issue in ALE, as in other etching processes, is aspect ratio dependent etching (ARDE) [2], which is the reduction of etch rates as the aspect ratio of a feature increases. One of the mechanisms linked to ARDE is the depletion of neutral species towards the bottom of a feature. This phenomenon has been investigated using a three-dimensional Monte Carlo method [3]. However, this method requires a complex setup and it is computationally expensive. For deposition processes, Knudsen diffusion [4] models provide analytical results and are actively developed. These models have been used for estimating surface parameters in some atomic layer deposition processes [5]. The Knudsen diffusion approach arises from physical considerations to the mass balance at each volume element. Alternatively, given isotropic reflections and particle source, the fluxes can be calculated exactly over the whole domain via the radiosity equation [6]. The radiosity approach requires the assembly and inversion of a matrix describing the exchanges, being notably unsuitable for low sticking regimes.

We propose a model extending the standard deposition Knudsen diffusion approach by including the direct flux from a particle source and a geometric factor to enable a more rigorous picture of ARDE in ALE. The inclusion of the direct flux is motivated by the radiosity equation, while avoiding the costly matrix inversion step. The geometric factor enables a more accurate description of the geometry by integrating over the whole feature at each volume element. We compare our extended Knudsen diffusion model against a reference radiosity model [6], achieving good agreement. Our results highlight one shortcoming of the standard Knudsen diffusion model: The flux near the bottom of a high aspect ratio feature is underestimated. We also show that the geometric factor describes the particle transport more accurately near the extremities of finite cylinders.

The financial support by the Austrian Federal Ministry for Digital and Economic Affairs and the National Foundation for Research, Technology and Development is gratefully acknowledged.

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