Multiscale Modelling of Physical Vapor Deposition for Semiconductor Thin Films: From Reactor Dynamics to Nanoscale Feature Evolution

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Physical Vapor Deposition (PVD) is an essential industrial process characterised by the physical sputtering of a target material and the subsequent deposition of the particles onto a substrate, such as a semiconductor wafer. This technique allows for the precise control of composition, thickness, and microstructure of the deposited materials.

The optimisation of semiconductor thin films necessitates a comprehensive understanding of how macro-scale operational parameters ultimately determine the final deposited film properties. This requires a computational framework capable of resolving phenomena across an enormous dynamic range, linking the *~50 cm* scale of the entire deposition chamber (where boundary conditions are applied) through the *~1 mm* shadow mask structural dimensions and further down to feature level of *~50 nm*, where deposition spots evolve. This endeavour involves bridging approximately 9 orders of magnitude in volume.

In this talk a multiscale simulation framework (Fig. 1 left) that connects the scale of the deposition chamber with the feature scale will be presented, explicitly accounting for shadowing effects and the role of the background gas (Fig. 1 right). Rarefied transport is modelled using Direct Simulation Monte Carlo (DSMC) to obtain energy- and angle-resolved particle fluxes at the substrate, which then serve as boundary conditions for level-set based feature-scale simulations. The framework is used to analyse not only local deposition profiles and step coverage, but also the spatial evolution of film composition across the wafer and within individual features.

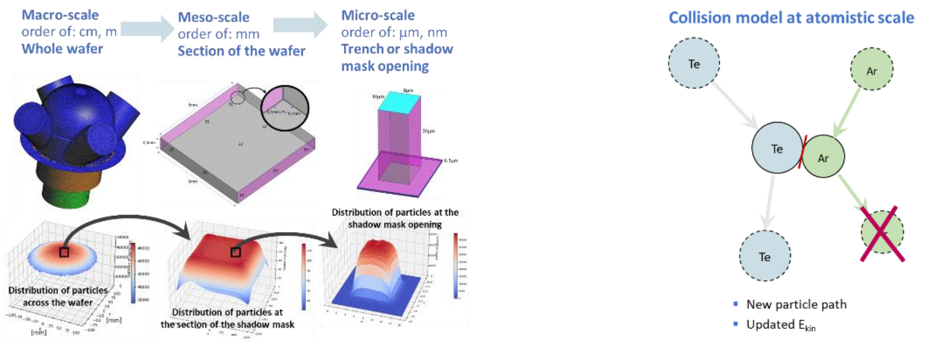

Figure 1. A multiscale simulation framework for PVD process modelling (left) and a collision model between material particles and background gas molecules (right).

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