Workshop »Digital Data creates value – recognising and exploiting opportunities«

Digital Vapor Deposition Processes: Multi-Scale Physics Modelling for Virtual Film Growth

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As the demand for advanced materials and miniaturization grows across various industries, the need for capable and efficient digital models for vapor deposition processes becomes increasingly important. These digital models create value by enabling process optimization, enhancing material quality, and reducing costs and business risk during process exploration. We present a multi-scale method for the simulation of physical and chemical vapor deposition processes in micrometer-sized structures, which incorporate physical process characteristics from the equipment scale and chemical kinetics from electronic modelling.

Our approach combines the numerical techniques of Kinetic Monte Carlo (KMC) sampling of individual adsorption events at the growing surface with Molecular Dynamics (MD) adsorption simulations, with a shared graph data structure of the surface mesh for efficiency. For large micrometer-scale substrates, workload distribution to thousands of CPU cores is achieved through an optimistic KMC formulation and parallel computation of MD adsorption events. Through additional geometric modelling of adsorption and growth mechanisms, coarser scales couple into the micrometer-scale atomistic model: Test particle raytracing in the surface mesh models the adsorption distribution in constrained microfeatures and small constrictions. The comprehensive model allows for the digital modelling and simulation of physical and chemical vapour deposition models, from the equipment to the resulting thin film.

Overall, efficient multi-scale physics models are powerful tools for optimizing functional thin film fabrication and driving further advancements in vapor deposition processes.