Multiscale Simulations of Thin Film Deposition Processes

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Thin film growths by Physical and Chemical Vapor Deposition (PVD and CVD) as well as electroplating are critical unit operations in fabricating mechanical, optical, and electronic devices. For example, layers of silicon, insulators, and metals are deposited and patterned by lithography and etching to form microelectronic circuits. Multiple layers of compound semiconductors (e.g., AlGaAs) with carefully controlled band structure and doping levels are synthesized by organometallic CVD or Molecular Beam Epitaxy (MBE) to yield lasers and detectors.

Similarly, deposition, patterning, and etching steps are used to realize microstructure composites, known as Micro-ElectroMechanical Systems (MEMS) for pressure sensors, accelerometers, and microfluidic applications. The deposition processes involve multiple length scales and different physical models may apply at these different scales (see Figure 8). The processes are used to define active regions on the micron (mechanical and electronic devices) to nanometer scale (optoelectronic devices) on substrates, which are held in meter-sized deposition chambers. Moreover, the underlying physical and chemical processes occur at multiple time scales. Individual diffusion processes and chemical reactions controlling the film growth and defect formation occur on typical atomic motion time scales of 10^{-13}s. In contrast, the growth of the active layer takes $\sim 10^{2}$s and the total processing time for a multilayer structure could be $\sim 10^{4}$s. We develop predictive, efficient models that bridge across multiple length and time scales by linking quantum chemistry, Molecular Dynamics (MD), kinetic Monte Carlo (kMC), and macroscopic finite element simulations. Application examples are drawn from chemical and physical vapor deposition of aluminum, organometallic chemical vapor deposition of AlGaAs, and electroplating of Cu. Experimental observations and quantum chemistry predictions of elementary surface reactions are incorporated into MD and MC simulations to provide new understanding of microstructure evolution. These computations are subsequently integrated into self-consistent feature and reactor scale models. Comparisons with experimental data are given at each length scale for the complete system.

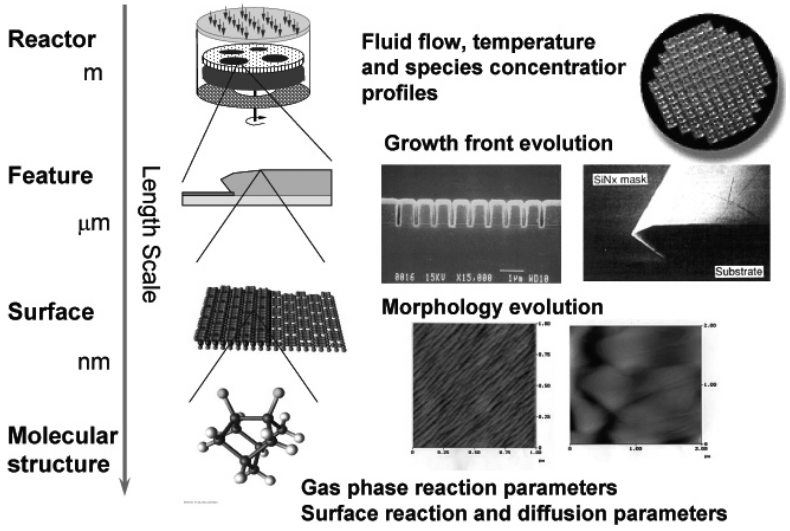

Fig. 8: Illustration of length scales involved in multi-scale simulations of thin film deposition processes.