

**A multiscale analysis framework for connecting chemical vapor deposition process conditions with product features and properties**

**Professor Andreas G. Boudouvis  
School of Chemical Engineering  
National Technical University of Athens, Greece**

A multiscale analysis framework will be presented for coupling macro- and micro-/nano-length scales in chemical vapor deposition (CVD) processes, used for growing thin films on wafers. A CVD reactor scale model (RSM), used for the description of the macro-scale reactive transport in the bulk, is implemented with a Computational Fluid Dynamics (CFD) code. It is coupled with a feature scale model (FSM), used for the description of the film growth and its profile evolution in the micro-scale features on the wafer; FSM is implemented by combining a ballistic model for the transport and the level set method for the profile evolution. Moreover, the RSM is coupled with the nanoscale, which refers to the surface level and the nanomorphology (roughness) of the film; it is simulated by a stochastic kinetic Monte Carlo (kMC) model which accounts for adsorption, diffusion and desorption.

The multiscale simulation enables predicting the effect of varying operational “macro”-parameters of the CVD process on the film growth rate and on important quantitative micro-/nano- film features and ultimately on their functional properties. Comparison of multiscale analysis predictions with experimental measurements of CVD of aluminum and iron will be presented.

[1] N. Cheimarios, G. Kokkoris and A. G. Boudouvis "Multiscale modeling in chemical vapor deposition processes: Coupling reactor scale with feature scale computations." *Chemical Engineering Science* **65**, 5018 (2010).

[2] I. G. Aviziotis, N. Cheimarios, T. Duguet, C. Vahlas and A. G. Boudouvis "Multiscale modeling and experimental analysis of chemical vapor deposited aluminum films: linking reactor operating conditions with roughness evolution." *Chemical Engineering Science* **155**, 449 (2016)

[3] I. G. Aviziotis, T. Duguet, C. Vahlas and A. G. Boudouvis "Combined macro-/nano-scale investigation of the CVD of Fe from Fe(CO)<sub>5</sub>." *Advanced Materials Interfaces*, in press (2017).