PRESENTATION

Prof. Henrik Pedersen

Linköping University | Professor

Henrik Pedersen received his M.Sc. in Chemistry in 2004 and his Ph.D. in Materials Science in 2008, both from Linköping University in Sweden. After a stint as industrial researcher at Sandvik Tooling Research and Development center in Stockholm, Sweden, he returned to academia and is today Professor of Inorganic Chemistry at Linköping University. His research is focused on understanding and developing new and better chemical vapor deposition methods by considering the time dimension in CVD, developing new precursors and new ways to use plasmas in CVD.

"In silico ALD – more bits and less pieces"

March 25, 2021 | 14:10 – 14:30

ALD presents a challenging, multi-scale modelling problem spanning at least ten orders of magnitude in both time and dimension; from the Ångström and picosecond scale of the surface reactions to the meter and seconds scale of the gas flows in the reactor. To establish a predictive modelling method for ALD, quantum chemical and DFT modelling of the surface interactions is connected to the gas flow patterns and gas exchange in the reactor via Computational Fluid Dynamics (CFD). We have recently shown how this connection is made in a continuous CVD process.[1] As the gas phase chemistry is (in the ideal case) negligible in ALD, it is a somewhat different process to model compared to CVD. Multiscale modelling of ALD is hampered due to the lack of CFD studies of ALD. We will discuss how predictive in silico ALD modelling could be done at the wafer scale.

[1] Danielsson et al. A Systematic Method for Predictive In Silico Chemical Vapor Deposition. J. Phys. Chem. C 2020, 124, 7725.