Industry lecture 2005

Årets "Industry lecture"

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25. 10 klokken 11.00. Auditorium 1, Kjemisk institutt, UiO.

Tittelen på foredrag:
'Modelling of multiscale systems with examples from chemistry'.

Forelesningen skal også holdes i Trondheim ved NTNU den 27.10.

Abstract

New applications in materials, medicine, and computers are being discovered where the control of events at the molecular and nanoscopic scales is critical to product quality, although the primary manipulation of these events during processing occurs at macroscopic length scales. This drives research in the creation of models for multiscale chemical systems that have length scales ranging from the atomistic to the macroscopic. The challenges to building such models include uncertainties in the physicochemical mechanisms as well as the values of thermodynamic and kinetic parameters, complexities in the simulation of model equations that can span the subatomic to the macroscopic scales, and the lack of direct real-time manipulations and measurements of most properties at the nanoscale during processing.

This presentation reviews the challenges in the modeling and simulation of multiscale chemical systems, and how these challenges can be addressed by the (1) design and implementation of high-throughput millimeter- and micrometer-scale chemical/electrochemical systems so as to highly excite the experimental input space, (2) extensive utilization of scanning probe measurements, (3) utilization of stop-and-repeat experiments, and (4) an iterative model-building procedure consisting of Bayesian parameter

estimation and hypothesis mechanism selection. The key ideas are illustrated by applications to two processes of importance to the semiconductor industry: (1) rapid thermal annealing to form ultrashallow junctions in advanced CMOS devices, and (2) the electrodeposition of copper to form interconnects in electronic devices. For ultrashallow junctions, the results provide specific recommendations for microelectronics tool manufacturers on how to optimize processes to produce shallower junctions. For copper interconnects, systems principles are used to gain fundamental insights into surface reaction mechanisms, and to move towards the rational design of new chemistries.

Se også siste KJEMI side 10.