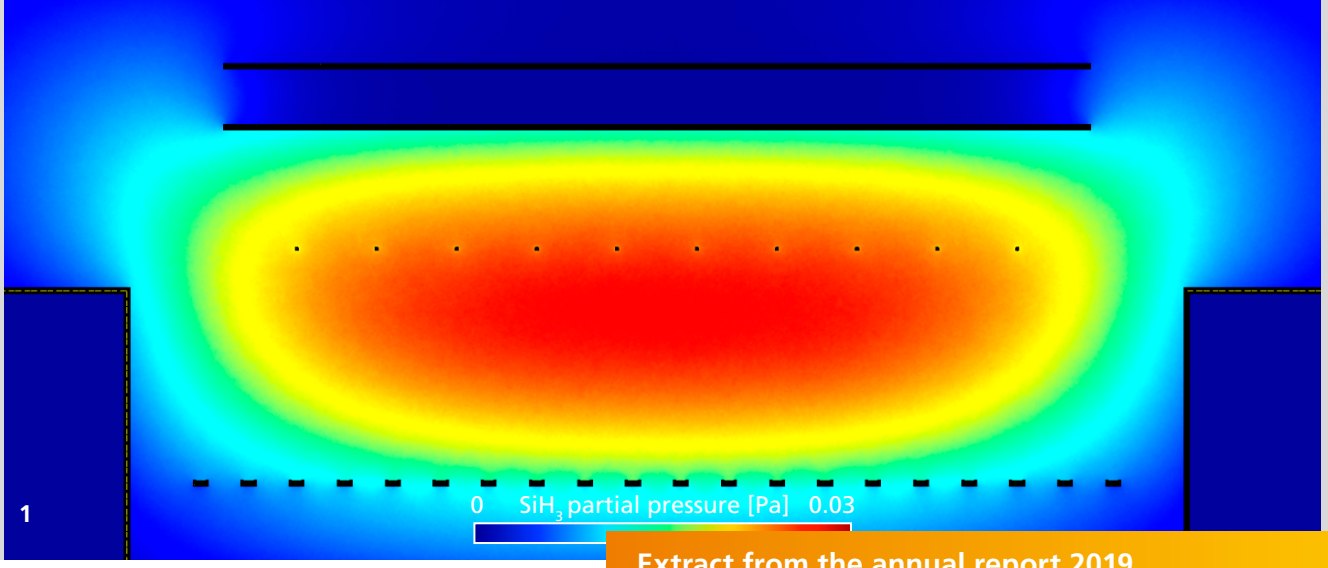

Extract from the annual report 2019
To the website: www.ist.fraunhofer.de/en.html

7 AFFORDABLE AND CLEAN ENERGY

DIRECT SIMULATION MONTE CARLO OF HWCVD SILICON DEPOSITION PROCESSES

Hot-Wire Chemical Vapor Deposition (HWCVD) processes provide the possibility to produce both amorphous and nano-crystalline doped and intrinsic silicon films with high rates up to 2 nm/s over large surface areas up to 800 x 665 mm^2. These processes have advantages to other deposition methods in that the film stress is significantly lower than with other technologies due to the absence of ion bombardment. However, the optimization of these processes can be a significant undertaking due to the relative complexity of the deposition. At Fraunhofer IST a full gas-phase and surface deposition simulation model of HWCVD silicon deposition processes, including silane (SiH_4) and hydrogen (H_2), was created as a tool to optimize film properties.

Simulation software

At the Fraunhofer IST the simulation group performs simulations of physical vapor deposition (PVD) and plasma processes using self-created software based on the Direct Simulation Monte Carlo (DSMC) method. Aiming for an increased understanding of silicon deposition processes, the HWCVD group partnered with the simulation group to develop an advanced simulation model of various HWCVD based silicon deposition processes.

Using the DSMC framework, this model was created with the goal to investigate how process parameters influence the structure of the as-deposited amorphous and nano-crystalline films. This new model implements both silane and hydrogen process gases, with hydrogen being used in deposition to influence the crystallinity of the resulting film. In addition, all major gas-phase and surface interactions of Si-species created during the deposition process were implemented in order to simulate how changing process parameters affect the concentration of specific gas-phase species, in addition to changes in surface-adsorption rates of these species.

Simulation confirmation and results

The new model is validated by an experimental parameter study. Measured data include deposition pressure, deposition rate (both film thickness and film mass deposition rates), in addition to mass-spectrometry measurements of silane utilization. After all simulated values agreed closely to the measured data, a series of simulation runs were made in order to simulate the effect of increasing hydrogen flow rate on the relative adsorption of specific silane species at the substrate position, in addition to the effect on the concentration of all major silane species in the gas phase.

The results of the simulation series confirm previous theory, which suggests that higher mobility species such as SiH_3 and Si_2H_4 lead to more crystalline films, whereas lower mobility species such as SiH, SiH_2, and Si_2H_2 lead to amorphous film growth. In addition, these results are confirmed by accordant experiments. Experimentally, an increase in either pressure or hydrogen flow leads to an increase in the resulting crystallinity of the film, where the simulation also shows a corresponding increase in SiH_3 and decrease in Si_2H_2 availability.

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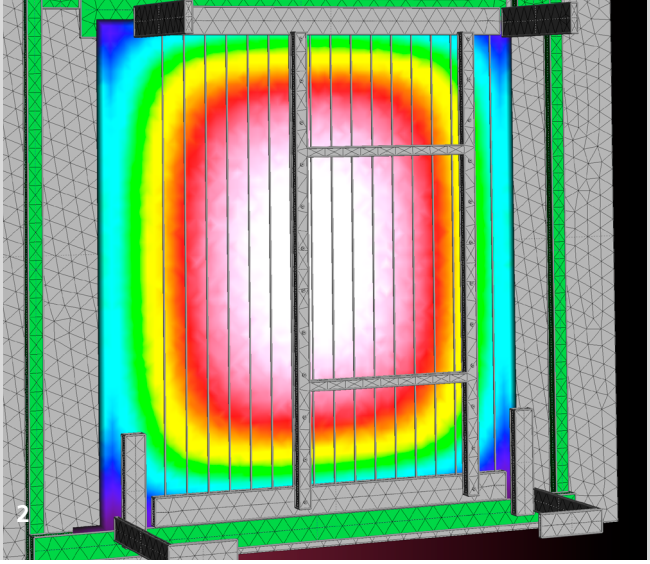
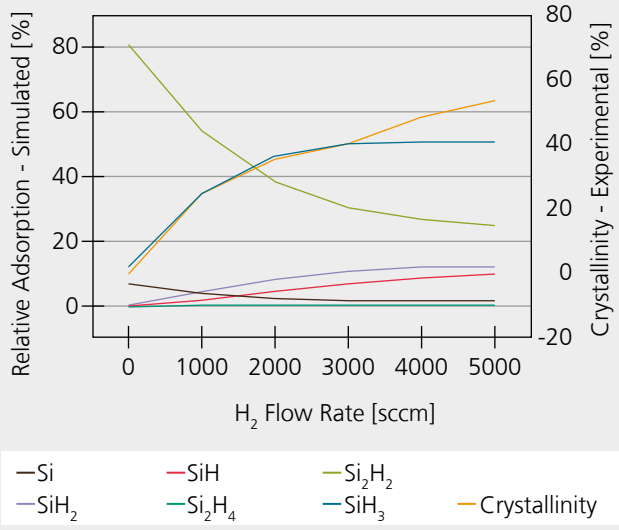
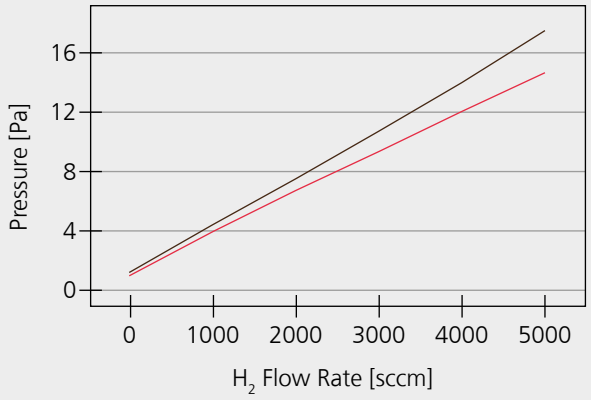




Simulated species adsorption at substrate as function of hydrogen.



Simulated partial pressure of SiH_3 species under steady-state process conditions.

1 *Simulated partial pressure of SiH_3 species under steady-state process conditions.*

2 *3D HWCVD chamber geometry used by Pflug et al.*

Outlook

This work provides many possibilities for process improvement in the field of silicon deposition by means of HWCVD, without the need for significant time and financial investment for wide-scoped test plans. With additional planned improvement involving the implementation of hydrogen-based surface etching reactions during the deposition process, the implementation of both phosphor and boron-based dopants, as well as an increase to surface-deposition model complexity, this model can provide even further insights into production-scale silicon deposition processes.

The project

This project was supported by the Fraunhofer Internal Programs under Grant No. MAVO 831 409.

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