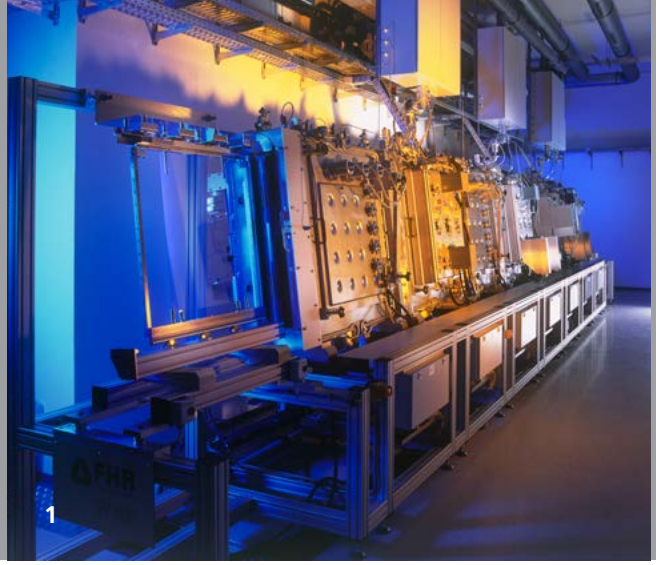

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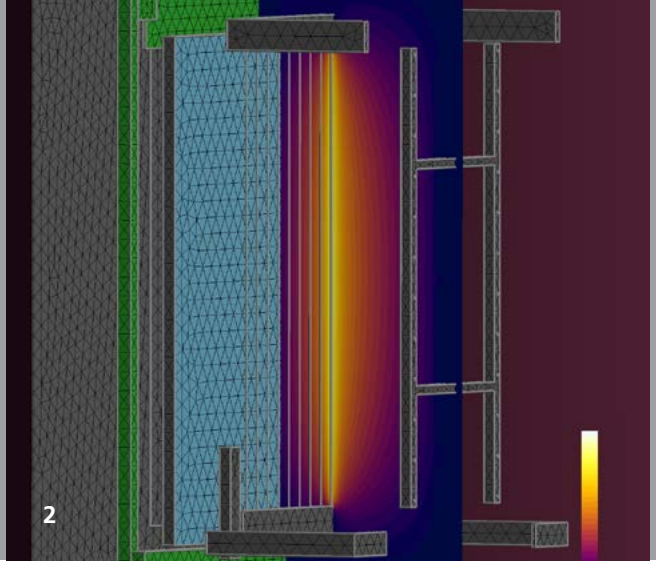

2

SIMULATION OF AN HWCVD PROCESS FOR SILICON DEPOSITION

Hot-wire chemical vapor deposition (HWCVD) is a promising alternative to plasma-based deposition processes for creating high-quality and defect-free coatings on large surfaces. At the Fraunhofer IST, this method is used in particular for the production of diamond- and silicon-based layers. With a simulation model the film thickness distribution and gas yield can be predicted in good agreement with experiment and thus HWCVD processes can be optimized with respect to layer thickness homogeneity and gas utilization.

Modeling the HWCVD process

Unlike other low-pressure coating processes there is no plasma discharge in the HWCVD process but instead current-heated tungsten wires are used to initiate the precursor decomposition reactions required for the coating. In order to deposit silicon on the substrate which is to be treated, silane (SiH_4), for example, is let into the reactor and at temperatures of about 2000 °C decomposed at the wires into silicon and hydrogen.

Modeling these processes calls for mapping of the gas flow and particle yield at the wires and walls. In the case of silicon layers with SiH_4 and NH_3 as process gases, deposition typically takes place in the pressure range of 1 to 10 Pa. The modeling processes which are based on continuum flow dynamics are inaccurate at such low pressures. For this reason the particle-based Direct Simulation Monte Carlo (DSMC) method is used at the Fraunhofer IST to describe the HWCVD process.

The Direct Simulation Monte Carlo method (DSMC)

In the DSMC simulation method individual representative gas molecules in the form of particles are considered. The movement of all gas particles, their sorting into ‘cells’, and the static treatment of particle collision within the same cell take place one after the other in short time cycles. In this way the Boltzmann transport equation is effectively solved by statistical methods.

The geometry of a coating chamber is represented in the form of meshed wall panels. In a movement step collisions between particles and walls are considered, the particles can be reflected or enter into chemical reactions with the material of the wall. With the DSMC method no 3D meshing of the total volume is thus required, only the walls need to be available in a 2D-meshed form. This considerably simplifies in particular the description of the thin heating wires, whose diameter is less than 1 mm. Otherwise, a 3D meshing of a volume of the order of magnitude of 1 m^3 while still taking into account details in the submillimeter range would be almost impossible.

Example: Silicon deposition on a steel substrate

Silicon deposition by HWCVD is simulated in the example of the in-line HWCVD unit at the Fraunhofer IST (see Figure 1).

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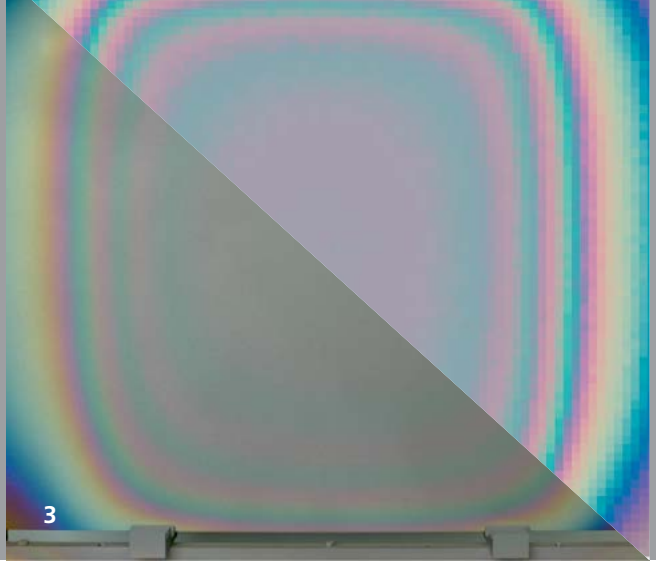
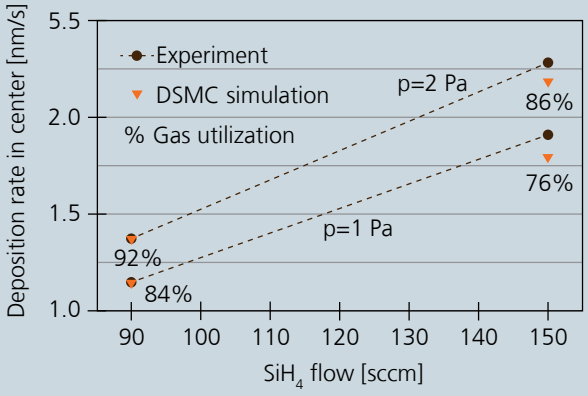


A coating chamber in this system consists of a gas distributor, a wire array between the gas distributor and the substrate, and the steel substrate itself, measuring 800 x 665 mm^2. The flow of SiH_4 used in the experiments is 90 sccm or 150 sccm while the process pressure is set at 1 or 2 Pa. In the model the wire temperature is 2100 °C – at this temperature there is a full decomposition of the silane. Despite the greatly simplified reaction model, there is good agreement between experiment and simulation (see Figure 3 and the graph below). Further details can be found in [Pflug2015].

Process parameters, simulated gas utilization and deposition rate compared with the experiment.



Further reading

[Pflug2015] A. Pflug et al.: Modeling of gas flow and deposition profile in HWCVD processes, Thin Solid Films 595 (2015) 266-271.

1 *In-line HWCVD facility at the Fraunhofer IST for depositing coatings containing silicon.*

2 *Model of an HWCVD chamber showing the Si-gas concentration (0 - 3.5%) in cross section.*

3 *Comparison of a photograph and a simulation of a coated metal plate showing the layer thickness profile and the resulting reflection color.*

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