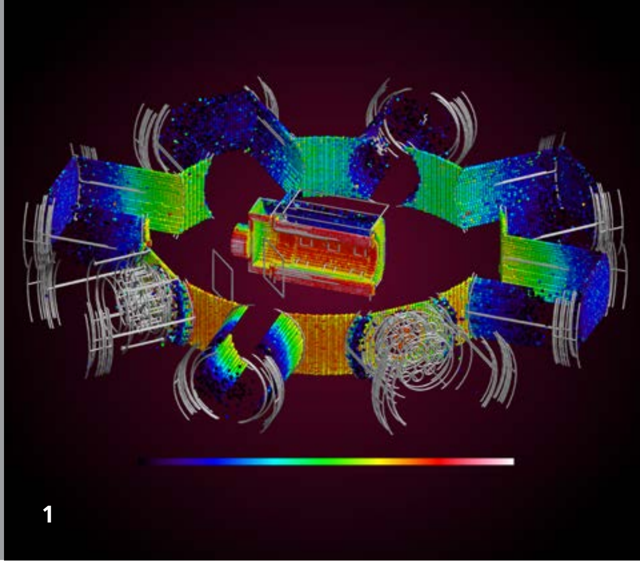
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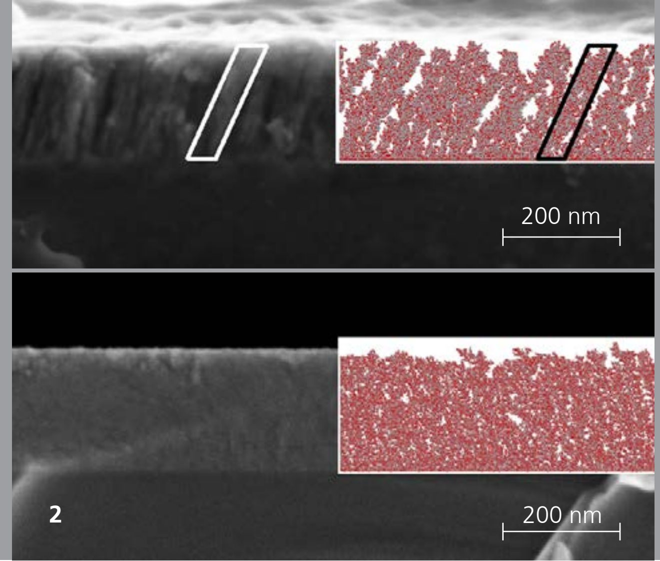

2

SIMULATION OF LAYER MORPHOLOGY AND LAYER STOICHIOMETRY

To successfully model plasma coating processes, processes must be considered on different scales of magnitude. In addition to the movements of the particles in the coating reactor, material growth at the molecular level is also important. The CORNET project »Computer-Aided Process Refinement for Intelligent Coatings« (or CAPRICe) combines flow and plasma simulations with layer growth models. Here the detailed growth conditions on the substrate are used as an input variable for subsequent simulation of layer growth. Predicting layer properties such as morphology and stoichiometry is possible with this concept of the »virtual coating system«.

Layer morphology

In order to compare the simulated and the experimental TiO_2 layer morphologies, the layer thickness profile in the system as well as the angle and energy distributions of particles arriving at different places on the substrate were first determined at the Fraunhofer IST. These angular distributions were passed on to the »NASCAM« software [Lucas2010] to be used as an input variable in modeling layer growth by the kinetic Monte Carlo method (kMC). In addition, a cross-section of the experimental layers was analyzed with the aid of a scanning electron microscope (SEM). Figure 2 shows that the simulation corresponds well with the experiment and that layer morphology on the substrate may vary depending on position.

Layer stoichiometry

In order to compare the layer stoichiometries of the simulation and the experiment – that is, the relative quantities of titanium and oxygen atoms – flow simulations (DSMC) were carried out for selected O_2 flow rates (2, 4, 6 and 8 sccm). Figure 3 shows the resulting partial pressure distribution for a flow rate of 2 sccm. Growth layer simulations (kMC) were also carried out over a wide range of flow rates. The layer stoichiometry was then determined and in addition layers made experimentally were investigated by Rutherford backscattering spectometry (RBS). The graph shows that there is good agreement between the results of all three methods.

Simulation expertise at the Fraunhofer IST

The parallelized simulation environment developed at the Fraunhofer IST has been optimized for thermal evaporation, magnetron sputtering and CVD processes in the low-pressure range. It enables the description of process kinetics in realistic 3D reactor geometries. Connecting up to additional simulation methods for layer growth means that intrinsic coating properties such as density, structure and optical properties can be predicted.

Further reading

[Lucas2010] S. Lucas, P. Moskovkin, Thin Solid Films 513 (2010) 5355-5361.

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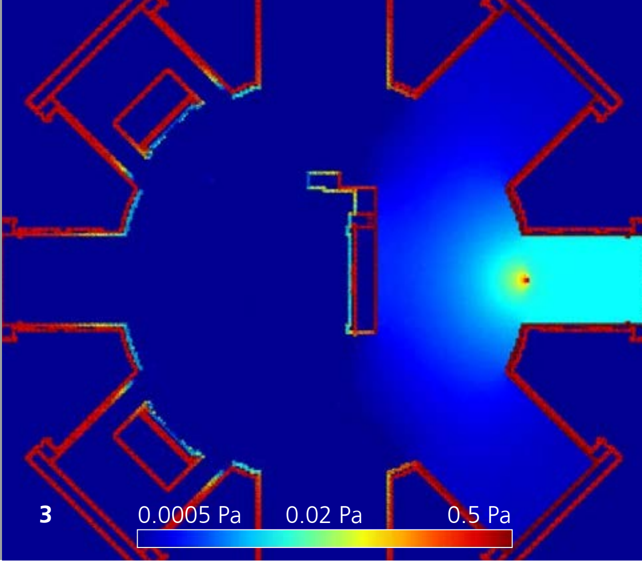
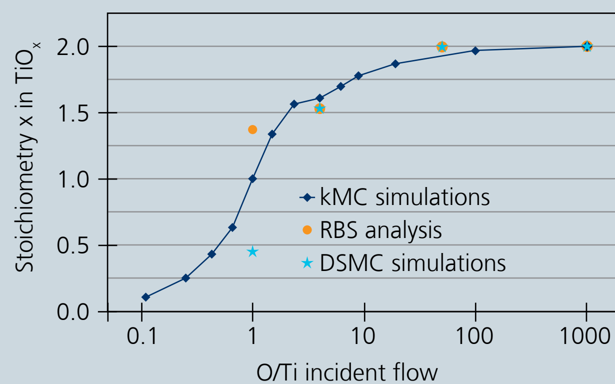


1 *Simulated layer thickness distribution in the sputtering reactor.*

2 *Comparison of REM images and simulated TiO_2 layer morphology (NASCAM software, University of Namur, [Lucas2010]).*

3 *Oxygen partial pressure distribution in the reactor at a flow rate of 2 sccm.*

Comparison of simulated and experimentally determined layer stoichiometries.



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