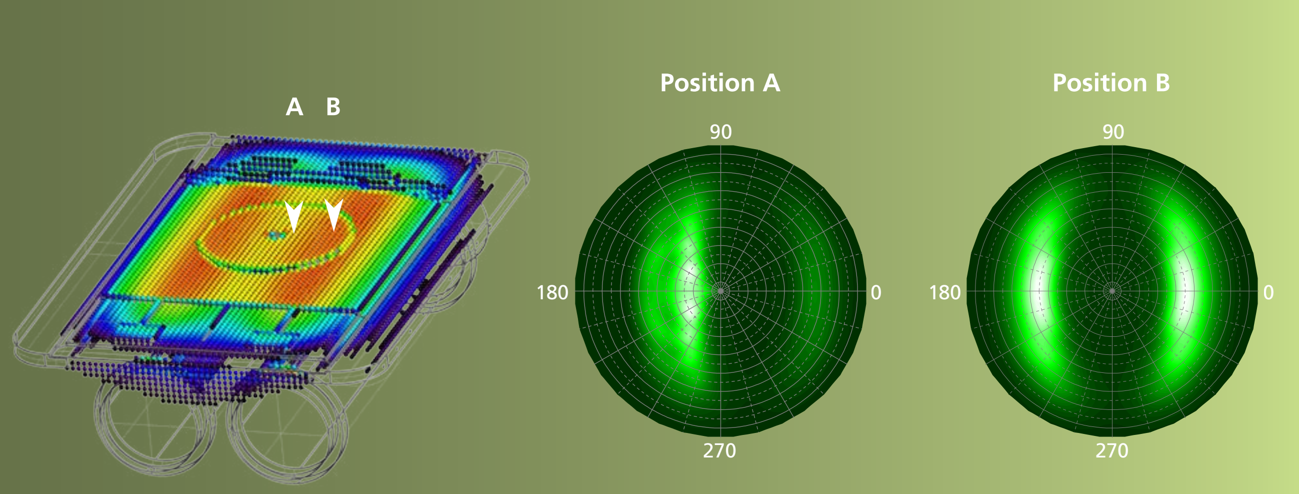

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MODELING OF THE COATING ON 3D COMPONENTS

Coatings on 3-D substrates are gaining increasing significance in various application areas. Examples are optical film systems on lenses, coatings onto curved vehicle windows or curved display surfaces. Via kinetic simulation methods, coating processes can be modeled in the low-pressure range and thus the film thickness profile can also be predicted. Unlike flat surfaces, for 3D substrates the substrate angle relative to the coating source also plays an important role. Therefore, for coating processes onto moving 3D substrates the movement sequence would need to be subdivided into small steps and a coating simulation would be required for each sub-step. Because this is extremely time intensive, a new method for accelerated modelling of the film thickness profile on 3D substrates has been developed at Fraunhofer IST.

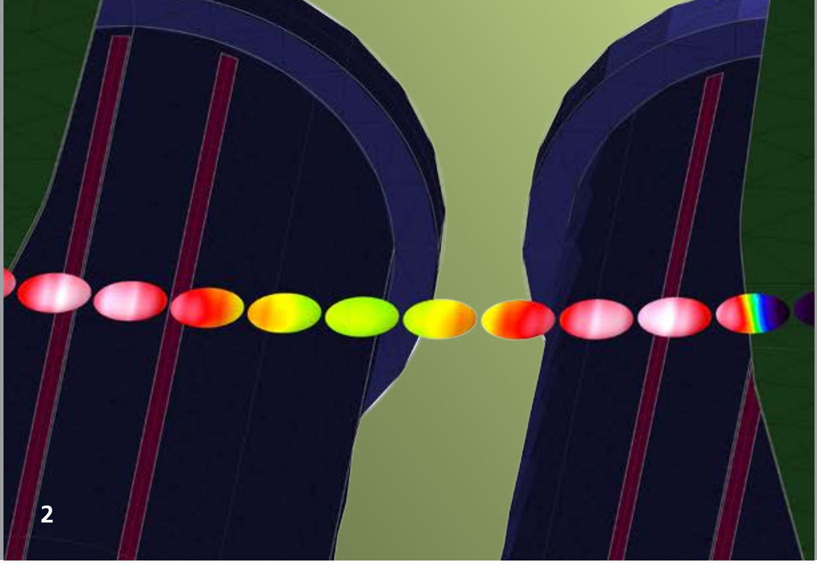
The simulation method

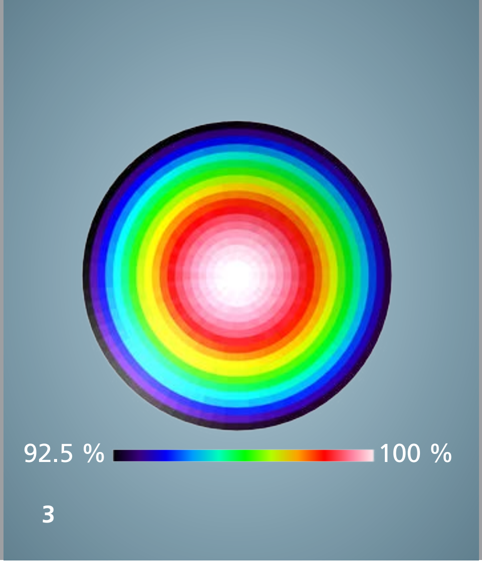
The "Direct Simulation Monte Carlo" (DSMC) method is suitable for modeling of flow and transport phenomena in low-pressure coating processes. This method describes the movement of molecules and atoms via representative simulation particles and presents a statistical approach for solving the Boltzmann transport equation. For example, DSMC is suitable for modeling the gas flow and film thickness profile in magnetron sputtering. In the case of moving 3D substrates, subdividing the motion sequence into many sub-steps, each of which requiring execution of the DSMC calculation, would be too time-intensive.

On the other hand, the newly developed simulation method requires only a single DSMC simulation. In this simulation, in a plane near the substrate the particle flow profile is sampled in lateral as well as in angular resolution and stored as intermediate dataset. Via a ray-tracing algorithm projecting the angular resolved flux density onto the substrate, this dataset allows for fast computation of the film thickness profile for 3D substrates in arbitrary positions. This is a viable approach because the scattering of sputtered particles in the gas can be ignored for the remaining minimal distance between sampling plane and substrate. Thus, this procedure enables a fast calculation of the film thickness profile for moving 3D substrates with fine resolution of the movement sequence. One example of location-resolved and angle-resolved particle flow distribution in a model of a sputter chamber is presented in Fig. 1.

Example: Dynamic coating of a lens

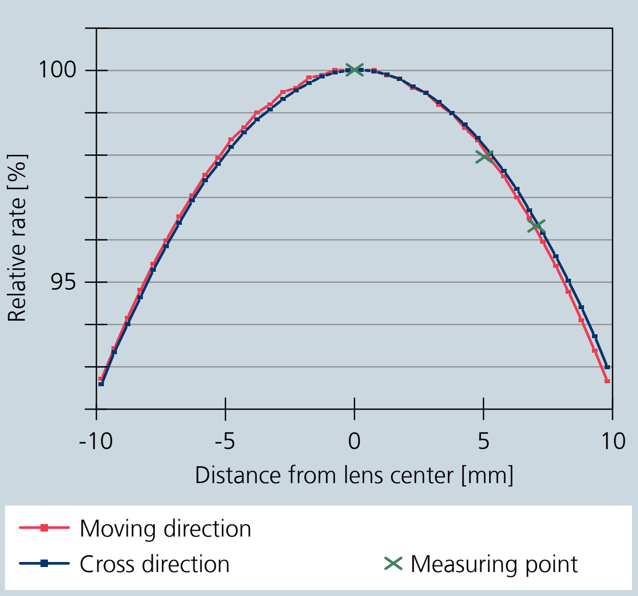
Starting with the particle flow profile shown in Fig. 1 and the selected aperture shape, the coating onto a spherical lens that is moved through the coating zone on a turntable can be quickly calculated via the ray-tracing method. The lens has a diameter of 20 mm and on the convex side a radius of curvature of 25.8 mm. Fig. 2 shows the partial film profiles on the lens surface for different positions of the movement sequence, as well as the overall profile resulting from the sequence. The discretization of the rotary plate movement occurs in the overall profile with an angular accuracy of 0.1°, the overall computation time is only a few seconds on a single CPU, and the resulting rate profile on the lens is consistent in good approximation with the measured data (see adjacent diagram).





The new, combined calculation method enables efficient calculation and optimization of film thickness distribution, and in principle this can be extended to any curved substrate shape.

Calculated film profile on the lens surface in the movement direction of the turntable (red), and in the transverse direction (blue) compared to film thickness measurements.



1 *Simulated particle flow profile of sputtered atoms near the substrate plane and angular distribution functions at selected points.*

2-3 *Partial film profiles of a lens at different positions and the accumulated overall profile.*

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