boltzplatz
numerical plasma dynamics

High-order 3D Plasma Simulation of a DC Magnetron

boltzplatz offers services around the simulation software PICLas, originally developed by the University of Stuttgart.

Particle-in-Cell

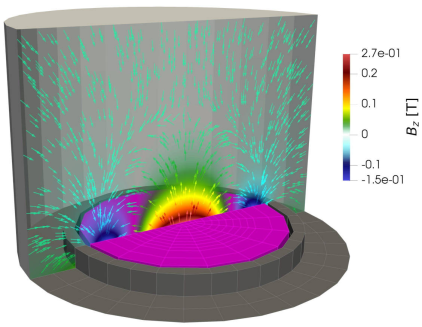
The Particle-in-Cell (PIC) method in PICLas self-consistently models a collisionless flow of charged particles under the influence of electromagnetic forces. To treat electromagnetic or electrostatic interaction, Maxwell's or Poisson's equations are solved with a high-order discontinuous Galerkin solver:

- Stand-alone 3D simulations or coupled with other particle-based methods
- Unstructured, non-conformal hexahedral meshes
- Efficient & scalable parallelization concept optimized for high-performance computing
- Automatic timer-based load-balancing strategy
- Choice between electromagnetic or electrostatic solution depending on the application

The PIC method can be coupled with other methods such as the Direct Simulation Monte Carlo (DSMC) or Monte Carlo Collisions (MCC) models to account for collision processes such as ionization and relaxation.

Direct current (DC) magnetron sputtering is an effective method used in thin film deposition processes to create, e.g., a metallic coating on an object. The material used for the coating is released or sputtered from a target (cathode) by bombarding that surface with energetic ions and then condensates on the substrate (anode) surface. To increase the deposition rate on the substrate, a magnet configuration is used to confine electrons in front of the target.

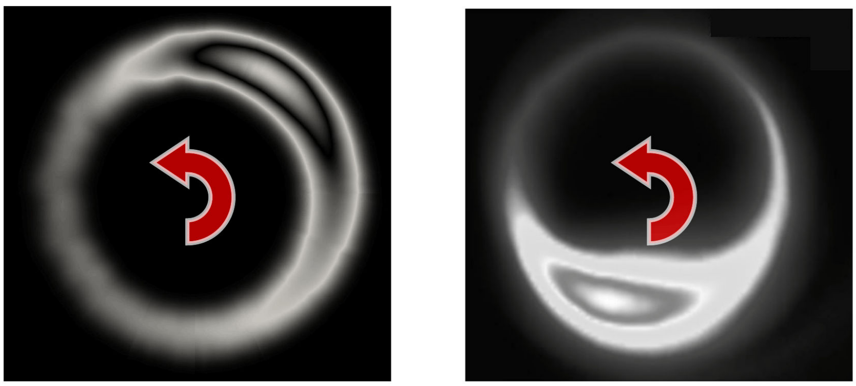
3D simulation setup



The simulation setup is adapted from an academic experiment. The simulation domain with target (pink) and magnetic field that is created by the coaxial permanent magnets below the target (outside of the simulation domain) is shown. The chamber is filled with Ar with a pressure of approx. $0.3\,\mathrm{Pa}$ and the voltage that is applied to the target is $-300\,\mathrm{V}$.

The Particle in Cell (PIC) method is applied to simulate the interaction between charged particles and electromagnetic fields and the collisions between the charged particles and the Ar gas are considered by the Monte Carlo Collisions (MCC) model, which assumes a background gas with constant properties over the course of the simulation.

Prediction of plasma instabilities: spokes



Typical physical phenomena that occur directly in front of the target surface are so-called spokes, waves of high electron density that rotate in a specific direction due to the trapped electrons in the magnetic field. The simulation (left) is compared with an experimental result given in the reference. For a given magnetic field distribution and applied voltage, the number of spokes and their rotating velocity depends on the background gas pressure.

Monte Carlo Collisions

The Monte Carlo Collision (MCC) algorithm offers a simple way to model particle collisions and chemical reactions in PICLas. For plasma simulations in combination with the Particle-in-Cell method, it can be utilized under the assumption of a background gas with constant properties, which is multiple orders of magnitude greater in density than the ionized species.

- Utilization of experimentally measured or ab-initio calculated cross-section data
- Modelling of the collision rates, excitation and chemical reaction rates
- Speed-up through Null Collision algorithm

Next to a constant background gas, results from a neutral gas simulation can be utilized as input for the plasma simulation. Additionally, a variable weighting factor allows the split and merge of simulation particles to efficiently model trace species.

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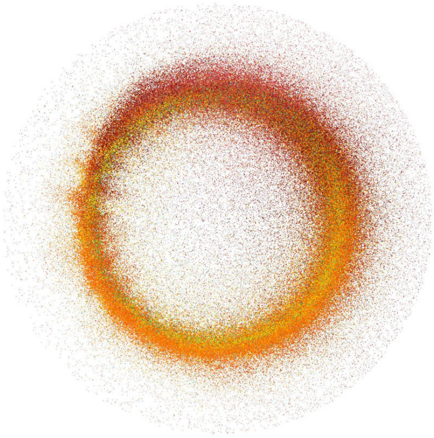
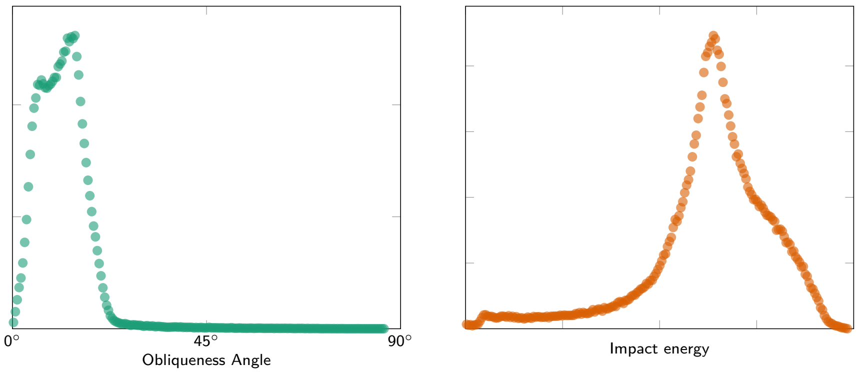
Prediction of impact rates



The impact pattern on the target reveals temporally and spatially resolved information regarding, among others, the impact momentum, energy and angle of ions and electrons. From these simulations, the erosion of the target surface can be determined and influences of the gas mixture and pressure, applied voltage, surface material, etc. can be quantified and used for optimization. In the picture above, the impact energy pattern of singly charged ions is shown and the effect of the occurring spokes can clearly be seen, which increases the impact energy of the ions at the current position of the spoke.

Impact distribution functions



Statistics from the target impacts give information about the distribution function of each species. The histogram plots above indicates the angle and energy bandwidth of the bombarding Argon ions. Again, the influence of the process parameters can be investigated by these simulations. Furthermore, details on the chemical composition of the plasma, the main chemical reactions that dominate the process and formation of radicals and tracer species are possible simulation outputs.

Sources:

- Pflug, A. & Vergöhl, M. (2019). Modelling of Thin Film Deposition Processes as a Service. *Proceedings of the 10th International Conference on Power Electronics for Plasma Engineering*, **73**(1-12), 978-83-930983-9-2.

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