8th Asia-Pacific Conference on Plasma Physics, 3-8 Nov, 2024 at Malacca

Erosion models and techniques to estimate model parameters for fusion applications

D. Reiser[1]

[1] Forschungszentrum Jülich GmbH, Institute of Fusion Energy & Nuclear Waste Management – Plasma Physics, Partner of the Trilateral Euregio Cluster (TEC), 52425 Jülich, Germany

e-mail (speaker): d.reiser@fz-juelich.de

Even if the magnetic confinement is of high quality, the vessel walls of a nuclear fusion experiment/reactor are exposed to a strong load from fluxes of high-energy ions and neutral particles. This results in significant material changes due to erosion processes, which depend on the characteristics of the ion fluxes and the specific wall material properties such as atomic mass, crystal structure, melting point and surface structure. The total amount of eroded particles, and thus also the life time of wall materials exposed to high-energy particle bombardment, changes significantly depending on whether the surface is polished, amorphous or structured. In addition, the irradiated surfaces can change over the course of exposure. The numerical simulation of these processes is time-consuming and complicated if an attempt is made to consider an extended surface and its morphological changes at atomic resolution. Fortunately, highly parallelized codes like ERO2.0 [1] are now capable of simulating such processes. However, even these high-performance tools are still too slow for an extensive parameter study for comparison with experimental results. Continuum theory [2-4] offers a simplification for the description of the surface dynamics. With the help of a global equation for the surface profile, the erosion processes and structure formation can be described numerically in a favorable way. The continuum theory can be understood as an averaged theory that avoids resolving the collision processes in the solid. Macroscopic parameters summarize the details on the microscopic scale.

We will show that machine learning methods can be used to determine the required model parameters from experimentally determined two-dimensional surface profiles. This is possible both for the case that the temporal development of the surface can be observed experimentally (via a series of snapshots of surface profiles [5]) and for the usual case that only a single snapshot is available [6]. Several approaches are discussed to cope with realistic data of ion beam experiments. Some basic ideas are similar to known methods from pattern recognition. By preparing a catalog of simulated profiles (training data), an ML algorithm for pattern recognition enables the identification of optimal model parameters that allow a simplified description of the erosion processes. Ultimately, machine learning processes avoid or greatly accelerate the tedious and often almost impossible adjustment of model parameters using trial-and-error methods. The characterization of different materials is made possible and the results can flow back into an atomic simulation to be used for predictive modeling of erosion processes in fusion devices.

References

[1] J. Romazanov et al.,Phys. Scr. T170, 014018 (2017)
[2] R. M. Bradley, and J. M. E. Harper, J. Vac. Sci. Technol. A 6, 2390 (1988).
[3] J. Muñoz-García et al., Phys. Rev. B 78, 205408 (2008)
[4] D. Erb et al., Phys. Rev. B 102, 165422 (2020)
[5] D. Reiser. Phys. Rev. E, 100, 033312 (2019)
[6] D. Reiser et al., submitted to Surf. Topogr.: Metrol. Prop. (2024)

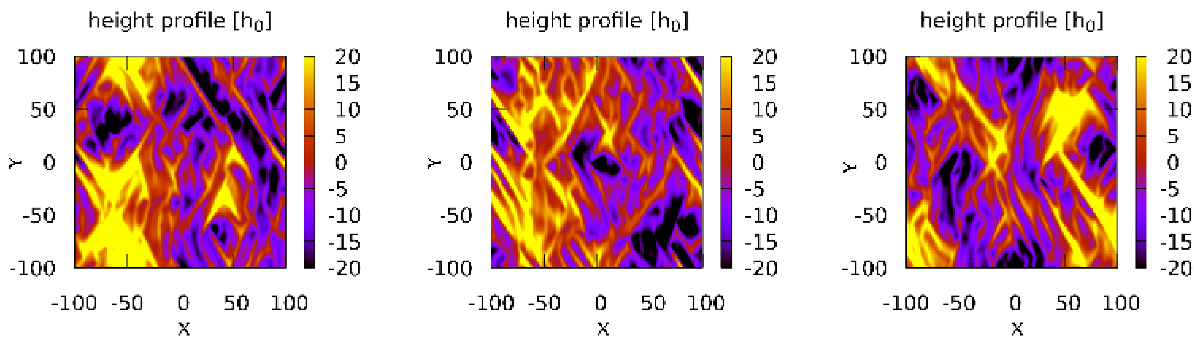

Figure 1. Examples of temporal morphological changes in synthetic data. Shown are the height profiles in x-y-plane in the course of exposition. The patterns appear similar to the human eye, which enables ML classification.