

# Model-based analysis of nanoscale interface evolution during spray coating

In modern thin film technology, spray coating plays a crucial role in fabricating flexible electronics and photovoltaics. The complex interface and multilayer structure are deduced by surface-sensitive scattering methods [1]. Spray coating was applied to create functional layers, from novel latex colloids to complex biomaterials templates [2,3]. There is a strong need to go beyond a one-dimensional analysis and to investigate the use of simulation-based analysis. The real-space structure is modeled (size and distribution of the nanostructures in three dimensions), the scattering pattern is calculated and compared to the experimental data. Hence, the goal of this project is to simulate the scattering pattern based on established algorithms and based on our results recently obtained [2,3,4]. The project includes image analysis, machine learning, supercomputing, as well as establishing reliable and feedback fitting routines. The simulations will be compared to previously acquired data [2,3,4]. Ultimately, the project participates in establishing a digital twin of the real experiments. The project is 50% physics and 50% computing.

## Literature:

- [1] S. V. Roth: "A deep look into the spray coating process in real-time—the crucial role of x-rays", J. Phys.: Condens. Matter 28, 403003 (2016)
- [2] J. Engström, C. J. Brett, V. Körstgens, P. Müller-Buschbaum, W. Ohm, E. Malmström, and S. V. Roth: "Core-Shell Nanoparticle Interface and Wetting Properties", Adv. Funct. Mater. 30, 1907720 (2020)
- [3] C.J. Brett, N. Mittal, W. Ohm, M. Gensch, L. P. Kreuzer, V. Körstgens, M. Månsson, H. Frielinghaus, P. Müller-Buschbaum, L.D. Söderberg, and S. V. Roth: "Water-Induced Structural Rearrangements on the Nanoscale in Ultrathin Nanocellulose Films", Macromolecules 52, 4721 (2019)
- [4] C. J. Brett, W. Ohm, B. Fricke, A. E. Alexakis, T. Laarmann, V. Körstgens, P. Müller-Buschbaum, L. D. Söderberg, and S. V. Roth: "Nanocellulose-Assisted Thermally Induced Growth of Silver Nanoparticles for Optical Applications", ACS Appl. Mater. Interfaces 13, 27696 (2021)

## Field

A3: Soft-matter sciences (application oriented)

## DESY Place

Hamburg

## DESY Division

FS

## DESY Group

FS-SMA

## Special Qualifications:

Programming experience is helpful

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