Workshop »Digital Data creates value – recognising and exploiting opportunities«

Advancements of Coatings simulations with Machine Learning Interatomic Potentials

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For coatings and fundamental material studies, simulations are a great tool to investigate details hard or impossible to access experimentally. The Laser Zentrum Hannover e.V. and partner institutes therefore developed a multiple scale model, named Virtual Coater™. In this framework the full coating process can be simulated by combining different methods for the material flow in the coating chamber, the atomistic growth, and the optical properties of the coating. For the atomistic growth two methods can be applied, namely molecular dynamics (MD) and kinetic Monte Carlo (kMC). While kMC can also model diffusion, the MD is more accurate and not limited to a fixed grid for atomic positions. However, so far the MD accuracy is still limited by hardware power and the choice of the interaction potentials. While potentials of e.g. the Lennard-Jones or Buckingham type can be computed fast, their accuracy is very rough. A completely new approach results from the use of Machine Learning Interatomic Potentials (MLIP). Here, an AI-based training algorithm is used to transform the quantum mechanical interaction potentials, which have a very high accuracy but require an extremely high computational effort due to the complex physics-based models and the extreme modeling involved, into a data-based model. MLIP allow for employing MD simulations with nearly quantum mechanical accuracy. These can be used to relax grown structures in an additional step or also for the growth simulation itself by use of massively parallel GPUs. Currently, the application of MLIP is still very much limited to exemplary studies in the context of university research. The implementation in the Virtual Coater™ in the context of the work in the cluster of excellence "PhoenixD" allows for the first time the application to real coating processes and the solution of questions from the experimental environment.

We compare the results of structures with MLIP-MD applied with structures from standard MD on the one side and quantum mechanically computed structures on the other side. The radial distribution function and coordination numbers are important benchmarks here. Further the resulting much higher accuracy of simulated structures, especially for stress or vibrational absorption are shown.