A novel coarse-grained model for the discrete element simulation of aggregated TiO$_2$ nanoparticle films

Oxide nanoparticle films produced by flame-based methods find applications in battery or fuel-cell electrodes, gas sensors, and catalysts. We have developed a coarse-grained contact model for the Discrete Element Modelling of TiO$_2$ nanoparticle films under mechanical stress. The particles can interact both via elastic sinter bridges or weaker capillary and solvation forces. The model’s mathematical terms and parameters are derived in a self-consistent and physically sound way from all-atom Molecular Dynamics simulations of interacting particles and surfaces. In particular, the nature of atomic-scale friction and dissipation effects is taken into account by explicit modelling of the surface features and water adsorbate layers that strongly mediate the particle-particle interactions. The predictive power of the model is validated against atomic force microscopy (AFM) and mechanical compaction experiments, revealing previously unknown details into the film restructuring due to the application of external loads.