Modelling and Characterization of Aggregated Nanoparticle Films

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The structure and mechanical properties of aggregated nanoparticle films and filter cakes are important parameters for many different fields. The high porosity of these films allows fluid molecules to access the high specific surface area of the nanoparticles in applications including catalysis. Percolation paths enable the transport of charges which is an important aspect in gas sensor design. For these films the mechanical stability against environmental stresses is important for many applications. In an earlier study, we could enhance the film stability by mechanical compaction. Using the Colloidal Probe Technique, we demonstrated an increase in the films Young's Modulus at increased compaction pressures.

The design of stable nanoparticle films with tailored structural properties, such as porosity, pore size distribution and percolation threshold, however, depends on the understanding of the rearrangement of such films.

Models for aggregated nanoparticle films allow to investigate the effects of mechanical stress on rearrangement of aggregates and film properties such as percolation, porosity and pore size distribution. Discrete element method (DEM) simulations can simulate stresses on millions of particles and therefore, allow to investigate the rearrangement of particle films in great detail.

Here we present a DEM based particle-particle contact model for primary particles of a few nanometers. The compaction of these films in the simulation resulted in porosities and pore size distributions matching the experiments. These simulations provide information on rearrangement and contact mechanics at the nano level of primary particles.