A new discrete element contact model to simulate the mechanical behaviour of TiO_2-nanoparticle films

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ABSTRACT

Controlling the agglomeration and dispersion behavior of oxide nanoparticles is key to technical applications such as catalysis, sensorics or hybrid materials synthesis. Especially in large-scale industrial process units such as filtering and fluidization, the contact forces between individual nanoparticles directly influence the process efficiency and thus, indirectly, the production costs. Often nanoparticle assemblies are processed or employed under normal ambient conditions, which implicates the presence of a layer of adsorbed water molecules on the nanoparticles' surfaces in contact with humid air. Numerous experimental and theoretical studies show that interparticle forces under ambient conditions depend on a non-trivial combination of particle size, shape, surface hydrophilicity and roughness[1,2,3]. However, predictive models to actively tune the interparticle forces are mostly limited to each single contribution and are often applied to model systems with little transferability to real material/adsorbate combinations, which is the reason for the actual lack of realistic contact models for the simulation of nanoparticles.

In our reseach we use the results of extensive all-atom molecular dynamic simulations and force-spectroscopy experiments[4] to unveil novel interaction force mechanisms for interparticle adhesion and shear. It turns out that the measured forces are highly reproducible by explicitly taking into account the surface-adsorbed water layer and by considering the solvation forces induced by the water structuring at the surface. However, all-atom simulations are limited to very small system sizes and time scales. For this reason, we incorporate our comprehensive contact models into well-established discrete element modeling software to investigate the mechanical behaviour of large nanoparticle films. With this simulation setup it becomes possible to directly compare the influence of ambient conditions, film porosity and connectivity on the experimentally observed mechanical and rheological properties of the films.

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