

Structural and rheological properties of a colloidal suspension using Molecular Dynamics-Stochastic Rotation Dynamics

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Self-assembly of mineral aggregates is a process of key relevance in nature and industry. A characteristic of self-assembly is the presence of a building block, with anisotropy in shape and interaction, which drives the formation of specific structures during aggregation. Rheological and mechanical response are strongly correlated to both the building blocks and the larger aggregates. A key example is calcium silicate hydrate (C-S-H), the binding phase of cement. Early models of C-S-H proposed a building block of a few nanometers, that forms larger units up to 100 nm [1]. Small angle neutron scattering techniques have resolved the building block as calcium silicate sheets, resembling narrow disks that stack together to form larger globules [2].

We explore the structural and rheological properties of a suspension of colloidal particles by means of computer simulations. Due to the size of the system, we focus on a coarse-grained simulation where particles have aspherical shape and anisotropic interactions. The fluid environment is taken into account using stochastic rotation dynamics (SRD), which includes hydrodynamic interactions, a key driving force in aggregation. We measure the shear viscosity using a reverse nonequilibrium method, and explore the dependence of the viscosity on the inter-particle interactions and the composition of the suspension. This investigation provides insight into the impact that organic additives have on surface functionalization and transport properties. The effective potentials used in the Molecular Dynamics-SRD simulations can be constructed from interactions obtained from full atomistic simulations, bridging molecular and mesoscopic scales.

[1] Jennings (2000), *Cem. Concr. Res.*, 30, 101-116.

[2] Chiang, Fratini, Baglioni, Liu & Chen (2012), *J. Phys. Chem. C*, 116 (8), 5055-5061.