Molecular Dynamics Simulations of Sodium Water Glass

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Basic sodium silicate can easily dissolve in water and forms water glass. The Water glass is used to make silica gel, in passive fire protection, to make cements, as lubricant for drilling, etc.. From view point of mineral science, water glass can be considered as analogue of aqueous fluids or wet melt. Structure of the water glass is not clearly understood but some results obtained by small angel X-ray scattering (SAXS) indicates that the oxide forms nano-scaled clusters. Gerber et al., (1994) reports that dilute sodium metasilicate water glass (> 6.5 mol/l) has only broad peak from near neighbor and Si-Si intermediate structure. However, water glass dried at ~323 K has the pre-peak that reflects ~ 1.0 nm ordered structure.

To reveal the actual structure that forms pre-peak of X-ray scattering, I performed force-field molecular dynamics simulations for sodium water glass system. The MD simulation appropriate method for study of structure of amorphous materials because it gives trajectories of each atoms in the simulation cells of each atom at any point in simulation time. MD simulations of sodium water glass consist of approx. 20,000 particles were performed using MXDORTO code (Noritake & Kawamura, 2016). I used the “dissociative” potential model proposed by Mahadevan et al., (2019), which can reproduce various properties of wet/dry silicate system and DFT calculation derived forces.

The simulated water glass (~approx. 15 mol/l) successfully reproduced the SAXS pattern which has pre-peak. The simulated water glass consists of nano scaled (~2.0 nm) Na_2O cluster, large sized silicate anion terminated by hydroxyls that surrounds Na_2O clusters, and interstitial water molecules. The contribution for pre-peak is mainly intra-cluster Na-Na structure.

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