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(GOMD-S4-075-2018) New Insights into the Condensation Kinetics and Structure of Sol-Gel Silicate Glasses

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The sol-gel method is an attractive technique to synthesize homogeneous glasses with high purity while relying on lower processing temperatures than in the melt-quench method. The sol-gel method can also be used to synthesize unusual glasses that are likely to be inaccessible from direct quenching. However, the role of the composition and concentration of the sol-gel precursors remain unclear. Here, based on reactive molecular dynamics simulations, we investigate the sol-gel formation of calcium silicate glasses exhibiting various Ca/Si ratios. The structure of the obtained sol-gel glasses is compared to that of their isochemical melt-quenched counterparts. The role of the fraction of Ca cations on the condensation kinetics is discussed.