GOALI: Impact of Mixed Network Formers on the Structure and Properties of Oxide Glasses

Jincheng Du (University of North Texas), DMR-1105219

Practical glasses are multicomponent and usually contain more than one glass-forming oxide such as silica, alumina, and boron oxide. Fundamental understanding of the mixed glass-former effect on the structure and properties of glasses is important to glass processing as well as their technical applications. In this project, we combine atomistic simulations and experimental studies to gain insights of the mixed glass-former effect on industrially-important glass systems. Based on well designed experiments and first principles calculations, we develop new potentials of a common functional form to capture the coordination variation and charge transfer for glasses with different glass formers. MD simulations are then performed to study the structure, diffusion and thermomechanical behaviors of these glasses. Industrial collaborator provides support of critical experiments and opportunity for students' interns. Model glass compositions are being studied by NMR and neutron/X-ray diffractions, which will serve as input for potential development and validation of simulated structure models.

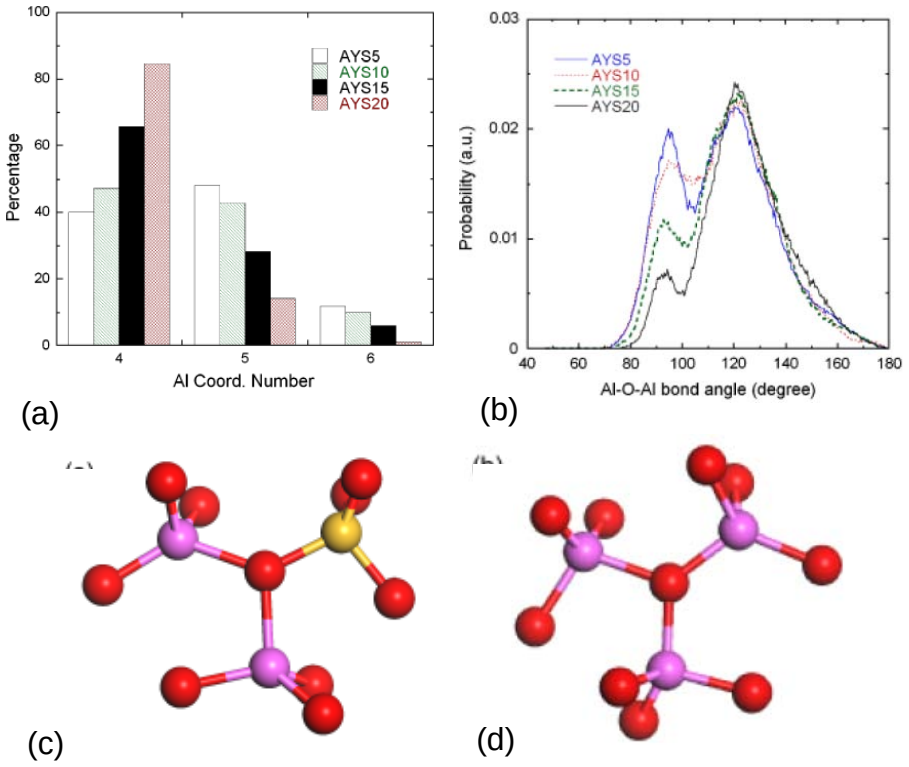

Fig. 1 (a) 4-coordinated Al increase and 5/6 coordinated Al decrease as SiO_2 concentration increases in aluminosilicate glasses from MD simulations. (c) and (d) snapshots of oxygen triclusters as a charge balancing mechanism in aluminosilicate glasses. Red ball: oxygen; organge ball: silicon; pink ball: aluminum.