Development of Mg/Al/Si/O ReaxFF Interatomic Parameters and Mechanical Properties, Damage Analysis, and Surface Analysis of S-glass Fiber

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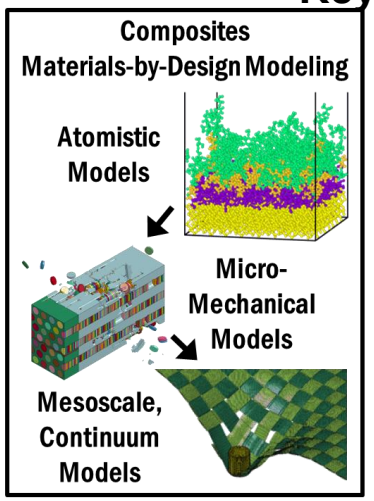
Key Goals and Technical Approach



- Composite property depends on its constituents: Fiber, Matrix, Interphase.
- Fiber/Matrix interphase property influences the overall composite quality and failure mode.
- Reactive MD simulation can simulate the accurate bond formation and breakage. It can predict the structural properties of interphase and interaction with composite constituents.

Mg/Al/Si/O ReaxFF Parameters

- Development of ReaxFF parameter set for description of S-glass.
- Development of ReaxFF parametrization automation algorithm.

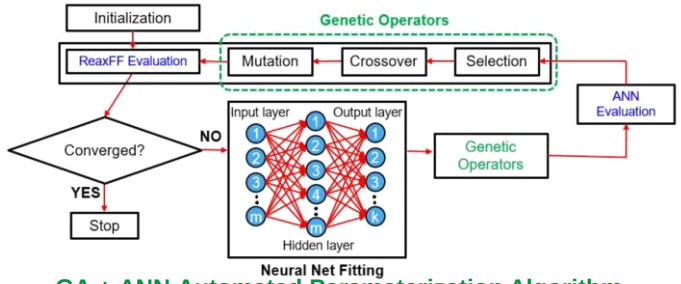
Mechanical Behavior of S-glass

- Quasi-static modulus and strength estimation from MD simulation.
- Atomistic origin of the mechanical response of S-glass and damage development.

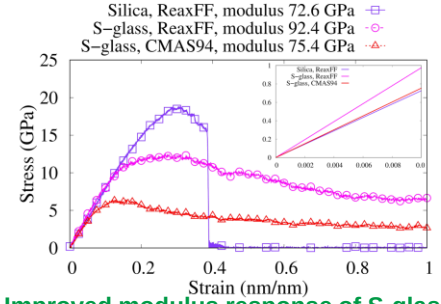
Surface Reactivity of S-glass

- Surface aerial density of hydroxyls on the S-glass surface.
- Categorization of hydroxyls and distribution of surface reaction site of S-glass.

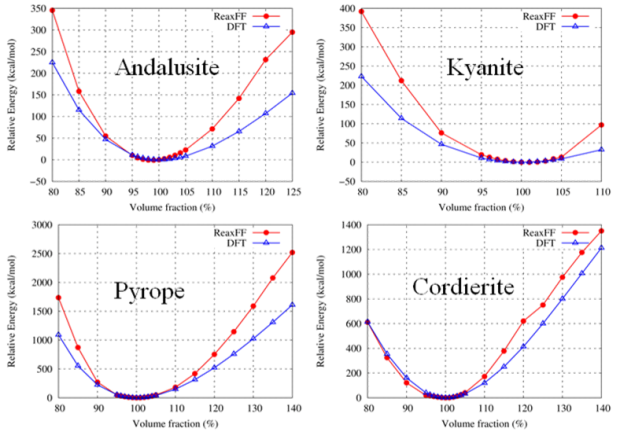
Development of ReaxFF Mg/Al/Si/O Interaction Parameters



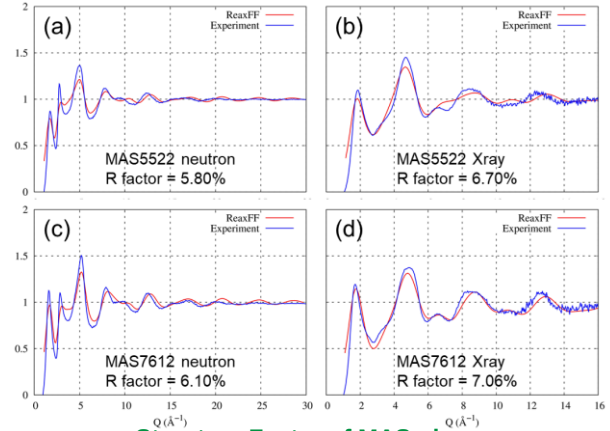
GA + ANN Automated Parameterization Algorithm [2021, Daksha et al.]



Improved modulus response of S-glass [2021, Yeon et al.]



Example equation of state energy curves [2021, Yeon et al.]



Structure Factor of MAS glass [2021, Yeon et al.]

- Genetic Algorithm assisted by Neural Network optimization algorithm enhance the efficiency of the parametrization. [2021, Daksha et al., Comp. Mat. Sci]
- Validation attempt, such as equation of state, modulus, and structure factor, from the newly developed ReaxFF Mg/Al/Si/O parameters agrees well with quantum scale simulations and experiment. [2021, Yeon et al., J. Phy. Chem. C]

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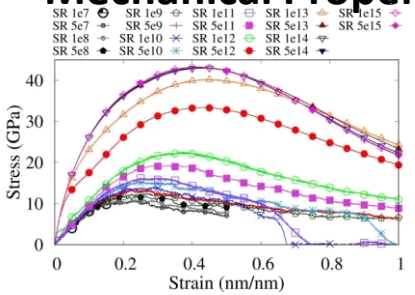
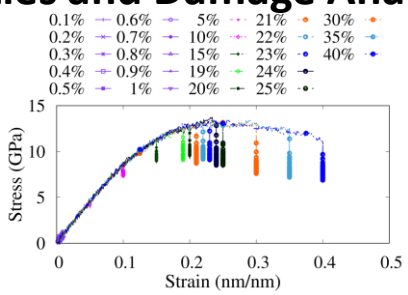
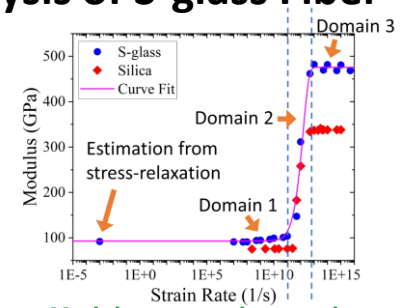
Mechanical Properties and Damage Analysis of S-glass Fiber



Stress-Strain curves of S-glass under 18 strain rates



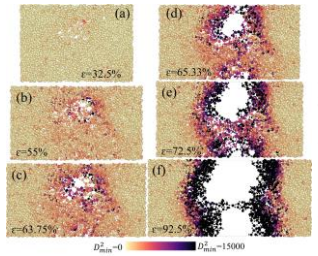
Stress-relaxation MD response of the S-glass



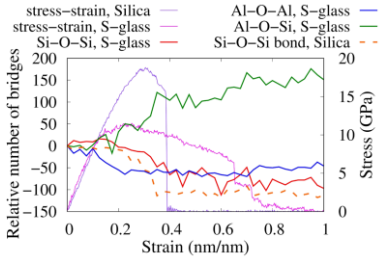
Modulus vs. strain rate plot of S-glass & silica glass

		ReaxFF, Multiple strain rate values at 1E-3/s	ReaxFF, stress-relaxation MD values at 1E-3/s	Experiment
S-glass	Modulus (GPa)	89.2	91.7	88~89
	Strength (GPa)	-	9.6	4.89
	Density (g/cc)	2.48~2.49		
Silica glass	Modulus (GPa)	72.2 [27]	72.2	69
	Strength (GPa)	-	15.9	3.20
	Density (g/cc)	2.20		

- Stress-Relaxation method can estimate the quasi-static modulus and strength of glass with reasonable accuracy from MD scale.
- Modulus and density S-glass and silica from ReaxFF MD matches well with experiment. Future effort will estimate the quasi-static strength with the influence of pre-existing crack.



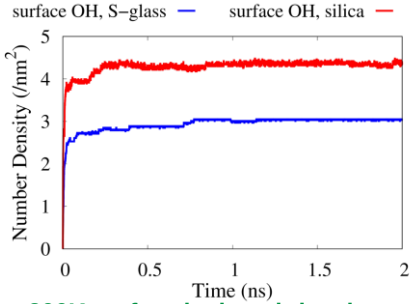
Void formation process of S-glass



Relative number of network former bridges of S-glass

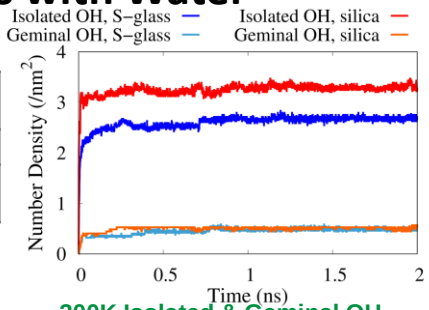
- Al-O-Si bridge and Mg-BO (bridge oxygen)/NBO (non-bridging oxygen) are responsible for the superior ductility of S-glass over silica glass.
- Results will be submitted in the Composite part B.

Surface Hydroxylation of S-glass with Water



Steady-state OH density	300K NVT MD	300K exp
S-glass	3.32	-
silica	4.41	4.2~5.7 [Zhuravlev]

300K surface hydroxyl density on S-glass & silica



300K Isolated & Geminal OH on S-glass & silica

- Areal number density of silica glass from ReaxFF is within the range of the experimental estimation.
- Spatial distribution of surface OH groups & surface-OH-water interactions will be analyzed.

Transitions (materials, codes/tools, legacy publications)

- GA (Genetic Algorithm) + ANN automated parametrization algorithm.
- Mg/Al/Si/O ReaxFF parameter set for the description of S-glass and silica glass, including DFT results.
- S-glass formation protocol and Stress-Relaxation MD simulation protocol.
- Two papers are published in peer-reviewed journal.
  - 2021, Daksha et al., Comp. Mat. Sci.
  - 2021, Yeon et al., J. Phys. Chem. C
- Mechanical properties and damage analysis of S-glass will be submitted in the Composite part B as legacy publication.

Future Plan

- Toughness of S-glass with defect & fracture energy analysis. (Dr. Chowdhury)
- Parametrization of Mg/Al/Si/O vs C/H/O/N interaction.
- Mechanical property-composition mapping of S-glass from atomistic scale.
- S-glsss/Epoxy interphase modeling.

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