

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

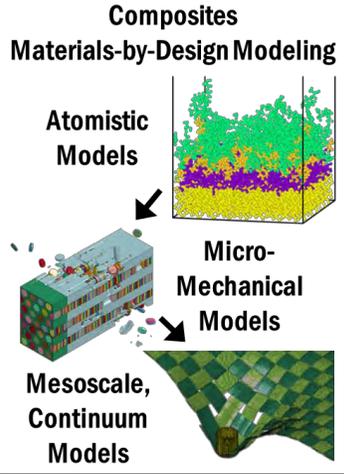
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## Key Goals and Technical Approach

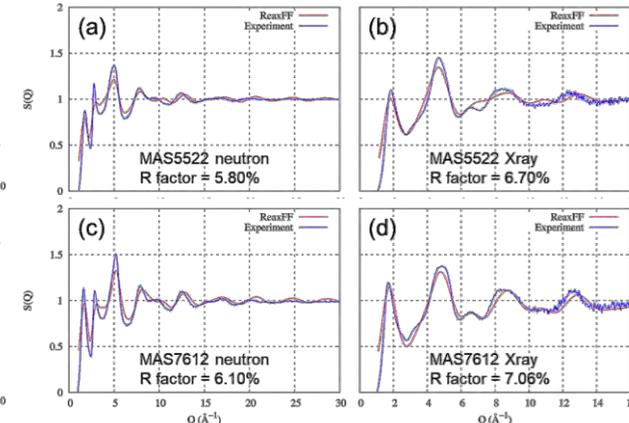
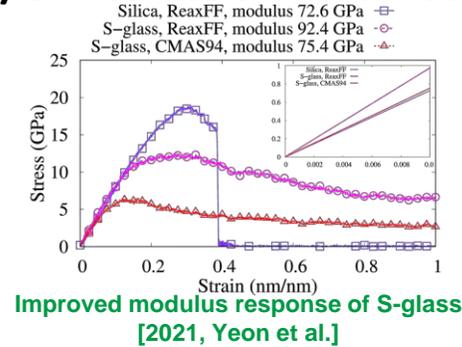
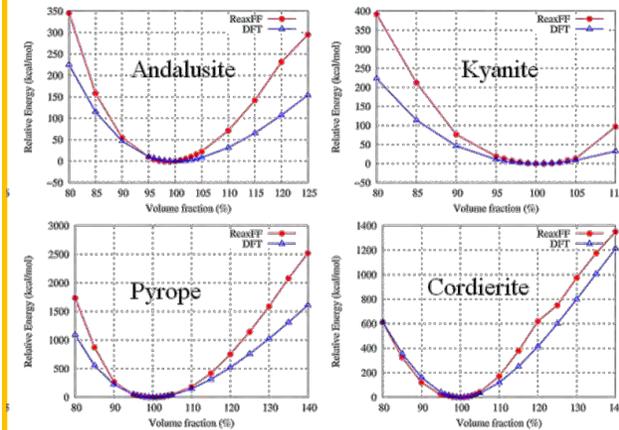
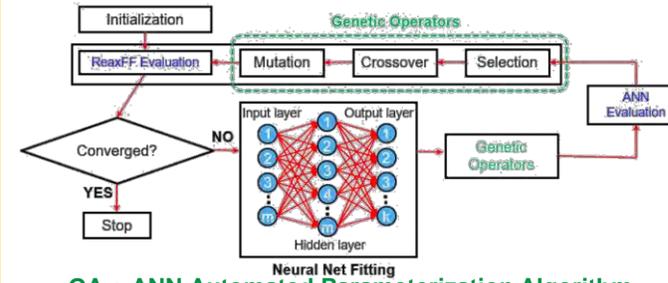
- ❖ Composite property depends on its constituents: Fiber, Matrix, Interphase.
- ❖ Fiber/Matrix interphase property influences the overall composite quality and failure mode.
- ❖ Reactive MD simulation can simulate the accurate bond formation and breakage. It can predict the structural properties of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



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



- ❖ 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]

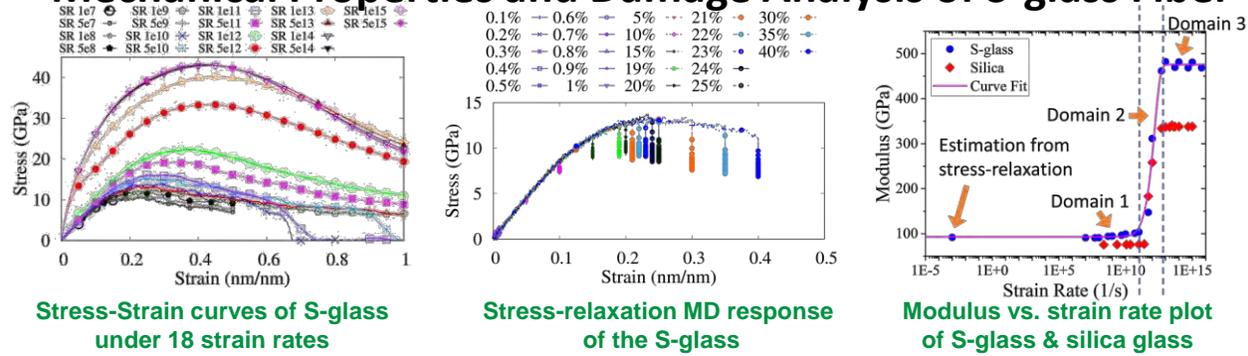
### Mechanical Behavior of S-glass

- 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

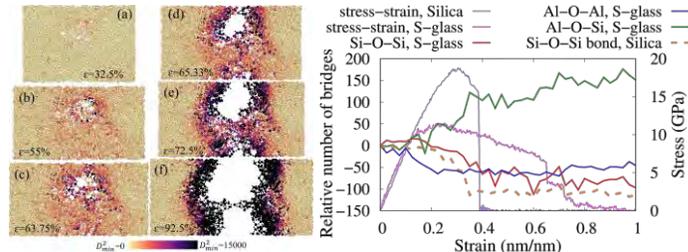
- Surface aerial density of hydroxyls on the S-glass surface.
- Categorization of hydroxyls and distribution of surface reaction site of S-glass.

# Mechanical Properties and Damage Analysis of S-glass Fiber



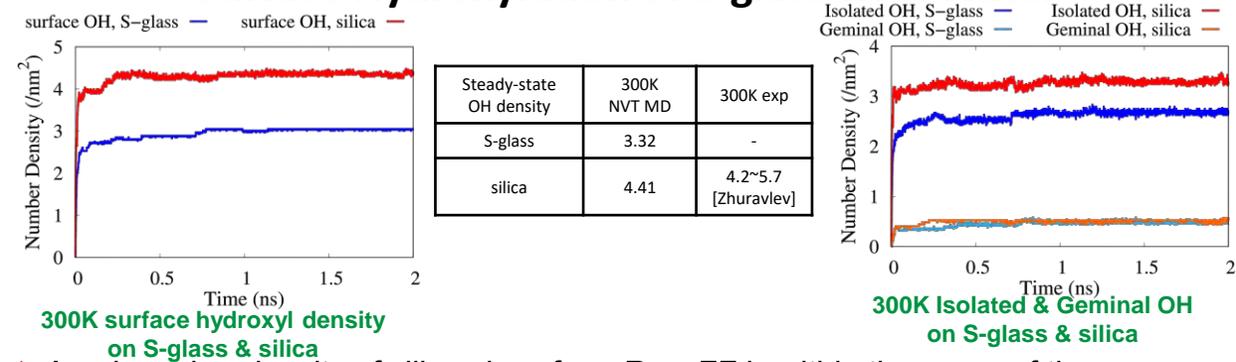
		ReaxFF, Multiple strain rate values at 1E-3/s	ReaxFF, stress-relaxation MD values at 1E-3/s	Experiment
S-glass	Modulus (GPa)	89.2	91.7	88~89
	Strength (GPa)	-	9.6	4.89
	Density (g/cc)	2.48~2.49		
Silica glass	Modulus (GPa)	72.2 [27]	72.2	69
	Strength (GPa)	-	15.9	3.20
	Density (g/cc)	2.20		

- ❖ 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.



- ❖ 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



- ❖ 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-glass/Epoxy interphase modeling.