Parameterization of ReaxFF Potential of Al/Si/O/Mg interaction for S-glass using Genetic-Algorithm assisted Artificial Neural Network

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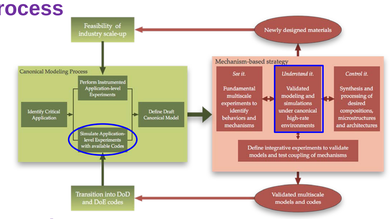
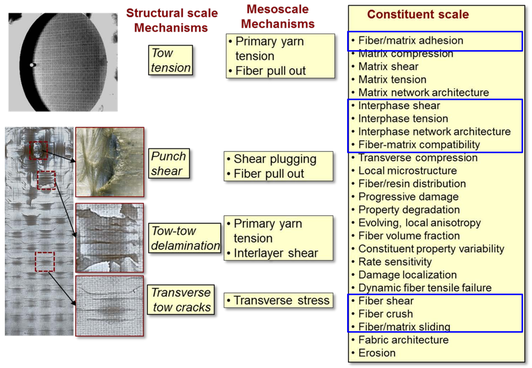
How We Fit

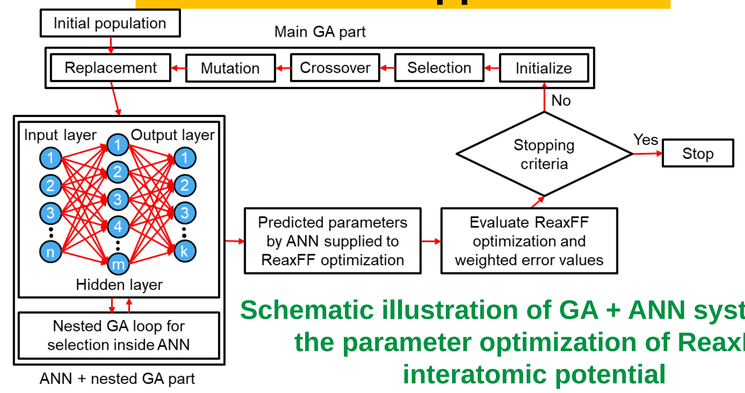
Materials-by-Design Process



Mechanism-based Approach



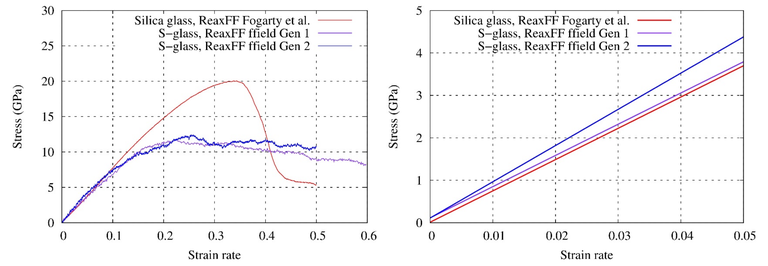
Technical Approach



Schematic illustration of GA + ANN system for the parameter optimization of ReaxFF interatomic potential

- Objective = find the best parameter set, which results the lowest possible weighted error values for training set.
- Artificial Neural Network (ANN) is widely known machine learning algorithm for categorization and prediction of future trend, Genetic Algorithm (GA) is an algorithm which could provide better input parameter set for ANN ➔ Accurate and efficient selection and prediction.
- Nested GA is applied for selection of parameter set for ANN.

Key Accomplishments/Path Forward

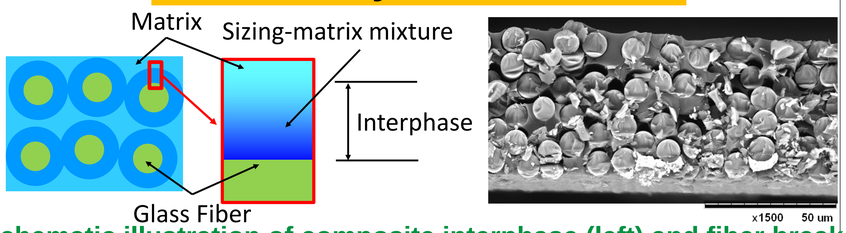


Stress strain curve 50% strain rate (left), 5% strain rate (right)

	Silica, Fogarty	Exp. Silica [2]	S-glass, ReaxFF Gen 1	S-glass, ReaxFF Gen 2	Exp. S-glass [2]
Young's Modulus (GPa)	74	69	74 (18% less than exp)	87 (3% less than exp)	88~91
Density (kg/m^3)	2.22	2.20	2.47 (1% less than exp)	2.51 (1% more than exp)	2.48~2.49

- Gen 2 forcefield parameters provide good correlation with S-Glass experimental results
- Long range interaction (high strain) behavior needs more attention.
- Gen 3 will be trained by completed DFT dataset.

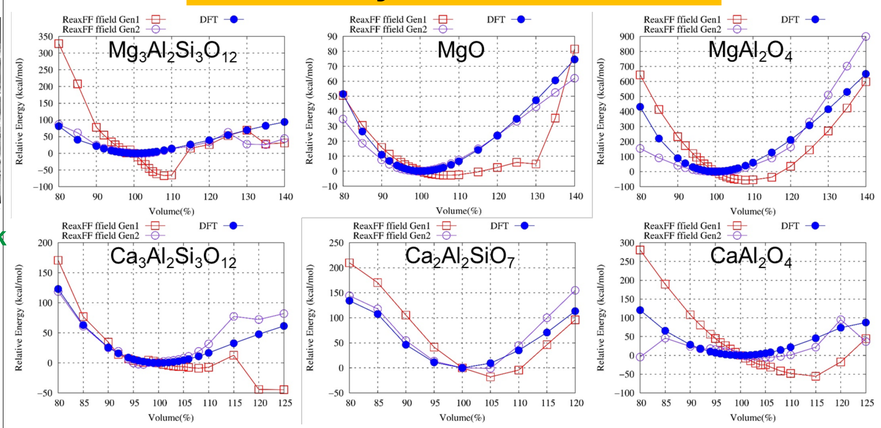
Key Goals



Schematic illustration of composite interphase (left) and fiber break and interphase debonding under punch shear (right, Haque et al.)

- Composites properties depend on the properties of fiber, matrix and their interphase. For glass fiber composite material, chemical reactivity of glass surface influences the strength of interphase. ➔ Important to understand the chemistry of glass fiber and its surface.
- It is very challenging to characterize the surface of S-glass fiber, effect of the sub-micro defect on fiber strength & toughness, and surface healing mechanism. ➔ Atomistic scale simulation is inevitable to understand and predict these properties.
- For the prediction of such properties with MD simulation, reactive interactive potential with proper parameters is inevitable. But no reactive interatomic potential for multiple oxide glass was developed so far ➔ Smart algorithm can enhance efficiency of parametrization.

Major Results



Example equation of state energy curves for S-glass ReaxFF ffield generation 1 vs S-glass ReaxFF ffield generation 2

- Gen 2 training sets (in progress) show improvements over Gen 1 results.
- Several regions require more fitting.
- More DFT (Density Functional Theory) simulations are in progress.

Transitions to ARL, within CMRG and to other CMRGs

- **Developed ReaxFF potential parameters and GA+ANN machine learning protocol will be transitioned to ARL.**
- **MD predicted properties of S-glass (for instances, constitutive law, surface defect effects etc.) will be used in other CMRG projects.**

Contribution to MEDE Legacy

- **New ReaxFF parameters for S-glass, will predict the fiber – matrix interaction and mechanical response of S-glass under various conditions more accurately, which can help to design better interphase.**
- **With new ReaxFF parameters for S-glass, virtual composition mapping will be enabled from atomistic scale point of view.**
- **New GA+ANN machine learning parametrization algorithm can be further enhanced.**

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