Studying the Structure-Property Relationships of Glass Systems Using Molecular Dynamics Simulations

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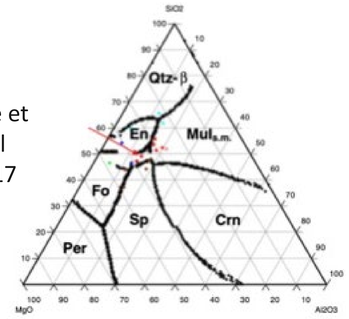
Introduction

- Interactions between atoms within aluminum oxide and magnesium oxide are critical to understand for the studying of the structure-property relationships of multi-oxide glass systems
- Using Molecular Dynamics (MD) simulations, we can develop composition mapping for multi-oxide glass systems

Ref. Belmonte et al. Chemical Geology, 2017



- Since the glass structure formation originates at the atomistic scale, we intend to study the structure-property relationships of glass systems using MD simulations
- MD simulations are carried out using Matsui and ReaxFF force field to model inter-atomic interactions
- By simulating with models of these compounds, it saves a lot of time, money, and effort which would have been spent in physical testing

Problem Specification

- Using MD simulations, we attempt to model aluminum oxide and magnesium oxide
- Aluminum oxide occurs naturally with a ranging density, so different models of this oxide will be generated
- MD models will be used to predict their structure and the MD predictions will be validated when compared with available experimental data

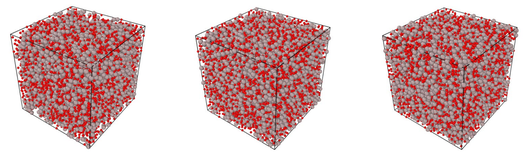
Methodology

- The software used in this research are Packmol and LAMMPS
- The first step of the procedure requires the initial configuration of the model to be generated by randomly packing the correct amount of atoms in a 3D box at low density using the Packmol tool
- Experimentally, aluminum oxide has a density ranging from 2.66 to 3.6 g/cm^3, so three densities were used to generate structures in Packmol: 3.0, 3.25, and 3.6 g/cm^3
  - Magnesium oxide has a density of 3.58 g/cm^3, so this was used for the Packmol simulation
- The generated Packmol models of aluminum oxide and magnesium oxide are used as inputs in LAMMPS simulations to make the glass structure by heating and cooling as in the outline below

- When the compounds are under NVT, there is a constant atom number, volume, and temperature
- When the compounds are under NPT, there is a constant atom number, pressure, and temperature
- This Matsui script follows the procedure necessary for glass formation
- Mechanical tensile loading with ReaxFF force field is performed to generate stress-strain response to predict mechanical properties

Results and Discussion

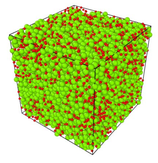
- After a series of trials in Packmol to determine the optimum tolerance to generate an accurate model, a tolerance of 2.25 was selected
- Using the tolerance of 2.25, aluminum oxide and magnesium oxide were modeled using the following densities:
  - Three densities of aluminum oxide:



3.00 g/cm^3: 4142 Al, 6213 O | 3.25 g/cm^3: 4488 Al, 6732 O | 3.60 g/cm^3: 4972 Al, 7458 O

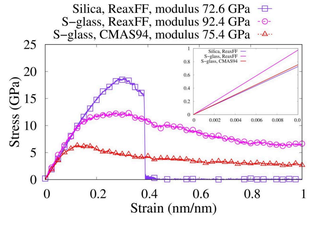
Al = Gray, O = Red

  - Magnesium oxide (3.58 g/cm^3), which consisted of 6165 Mg atoms and 6165 O atoms:



Mg = Green, O = Red

- Packmol models with randomly packed atoms are used as input in LAMMPS simulations to make the glass structure by heating and cooling as the outline depicts in the Methodology section
- The glass formation process is in progress. When it is complete, the developed model will be used to predict stress-strain responses like the following figure (obtained from Yeon et al.) to determine the mechanical properties of the systems:



Summary and Conclusion

- Modeling aluminum oxide and magnesium oxide is critical in determining the structure-property relationships of glass systems, as these oxides are major components of the systems.
- By using the data obtained through this research, the atomic interactions within multi-oxide glass systems can be better understood.
- Molecular Dynamics modeling can be used to identify and design optimal glass structures that can later be manufactured.
- MD simulations can also guide manufacturing processes.

References

(1) *Belmonte, Donato; et. al. The system MgO-Al_2O_3-SiO_2 under pressure: A computational study of melting relations and phase diagrams. Chem. Geol. 2016*

(2) *Yeon, Jejoon; et. al. Development of Mg/Al/Si/O ReaxFF Parameters for Magnesium Aluminosilicate 2 Glass using Artificial Neural Network Assisted Genetic Algorithm*

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