First-Principles Simulation and Visualization of Model Basalt Melt Structure

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Acknowledgement:
Outline

• Motivation
• Simulation
• Visualization
• Structural Analysis
• Conclusion
Motivation

• Basalt model is a major magma forming silicate melt
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• Knowledge of melt properties to understand transport and generations of magmas

  Volcanic eruptions

  Partial melts at ULVZs

• Early magma ocean

  Largely molten Earth in it’s early history
Motivation

• Melt properties are key to modeling the geological processes

  ✓ Wide range of melt properties to study...
  ✓ Focus on Structural properties which control other properties

     Radial distribution function, Bonds, Coordination numbers, Clusters, Rings
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- Complex system than previously studied systems such as along MgO-SiO$_2$ join:

  Model Basalt Liquid:

  64% mol. Diopside (CaMgSi$_2$O$_6$) + 34% mol. Anorthite (CaAl$_2$Si$_2$O$_8$)
Motivation

• HOW?
  ✓ Simulation
  ✓ Visualization
Simulation

• First principles molecular dynamics simulation

  ✓ Positions(trajectories) data by integrating Newton’s equation of motion

  ✓ Inter-atomic forces are obtained from density functional theory used for electronic-electron interactions
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• Super-cells consisting of 224 atoms(small system) and 488 atoms(large system)

• Time step = 1 femtosecond;
  Run duration of few tens of picoseconds
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• Simulations at different volumes covering wide ranges of pressure and temperature
Scientific Visualization

- Process of mapping complex data/information into visual forms or pictures or images generated by modern computers.

- Visualize the time-varying 3D scattered data from simulations

- Space-time multi-resolution visualization to gain insight into the structural and dynamical behavior using AtomViz.

*Atomistic visualization: Space-time multiresolution integration of data analysis and rendering.*

*J. Mol Graph. Mod., Bhattarai and Karki 2009*
Data: Position-Time Series

Model Basalt Melt

224 224 1
0.1507000E-08 0.1507000E-08 0.1507000E-08
5000.00000000000

Model Basalt
Config = 1
0.85733188 0.33764890 0.77924075
0.67213505 0.87220657 0.67834759
0.44961485 0.52760553 0.21170680

........

Config = 2
0.85697674 0.33850686 0.77965114
0.67177580 0.87168654 0.67908078
0.44779337 0.52724704 0.21138675

........

Species File

#AtomicName AtomicWeight StartIndex EndIndex
Ca 20 0 21
Mg 12 22 35
Al 13 36 51
Si 14 52 95
O 8 96 243
Rendering Atomic Data

Pathlines showing the atom trajectories for complete data for $V_x$ at 3000K [LEFT].

Instantaneous configuration of the system [TOP].
Partial radial distribution function -

\[ g_{\alpha\beta}(r) = \frac{1}{4\pi\rho_{\beta}r^2} \left[ \frac{dN_{\beta}(r)}{dr} \right] \]

\( V_x \) (red)

0.7\( V_x \) (green)

0.55\( V_x \) (blue)

all at 3000K.
With increasing temperature/pressure, peaks become shorter, wider and less symmetric.
Coordination Matrix Plot

\[ C = 4 \int_{r_{\text{min}}}^{r} r^2 g(r) \, dr \]

Color of centered spheres encodes coordination value.
• Al-O and Si-O coordination information is represented by color coded polyhedra.

• Ca-O and Mg-O coordination information is represented as ball-and-stick.
  
  Calcium (large sphere)
  Magnesium (medium sphere)
  Oxygen (small sphere)
Mean coordination for cation-anion and anion-cation pair decreases with increase in volume (decrease in pressure).
- Abundances of Si-O(solid)/Al-O(dotted) and O-Si(solid)/O-Al(dotted) coordination species
- Plotted as a function of compression(volume).
• Cluster of single Ca, Mg, Al, and Si and atom with O atoms at:
  \[ V_x, 3000K \text{ [Top row]} \text{ and } 0.55V_x, 3000K \text{ [Bottom row]} \]
Coordination Increase: Mechanism I

NBO + $2Si^n \rightarrow BO + z_{+1}Si^{n+1}$

- Coordination increase through transformation of non-bridging oxygen (NBO) to bridging oxygen (BO)
- A four-fold (cyan sphere) Si atom becomes a five-fold (blue sphere) by bonding with NBO, which then becomes BO (yellow sphere)
Coordination Increase: Mechanism II

Model Basalt melt at Vx and 3000K

\[ \text{BO} + _2\text{Si}^n \rightarrow \text{O}_3 + _{z+1}\text{Si}^{n+1} \]

- Coordination increase through the BO
- A five-fold (blue) coordinated Si atom turns into a six-fold (purple) coordinated Si atom after bonding with BO, which then changes to three fold (green sphere)
Visualizing Model Basalt Melt

FPMD position time data for Vx 3000K [LEFT] and 0.55Vx 3000K[RIGHT]

- Si-O and Al-O coordination as polyhedra
- Ca-O and Mg-O coordination as ball-and-stick
- Color-coded pathlines for mobile Ca and Mg atoms
- Ca(large sphere), Mg(medium sphere) and O(small sphere), all color coded
Conclusion

• Visualization of simulated data allows us to understand the complex structure of silicate melts.

• Visualizing position-time series is more than just direct rendering of data.

• Coordination environments consist of a rich variety of species.

• Melt structure substantially changes on compression
  Mean coordination numbers increasing with pressure.