Emerging Nano and Advanced Materials

Development of a transferable inter-atomic potential for NABS glasses

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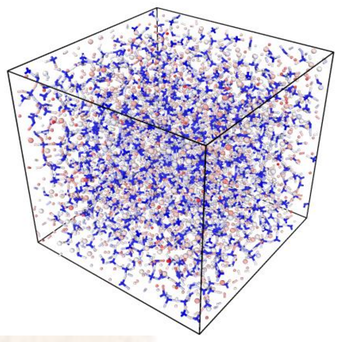
Abstract

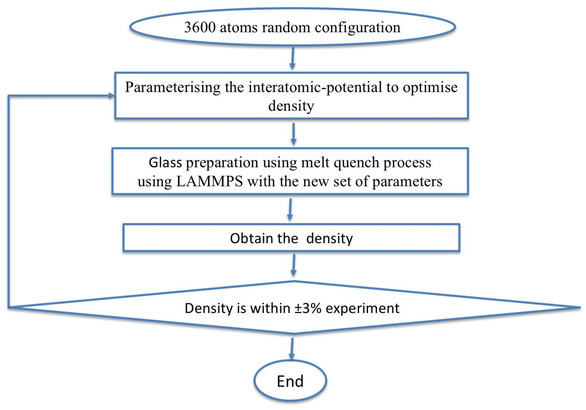
- Boroaluminosilicate glasses are used for: smart phone protective screens to nuclear waste immobilization.
- MD simulation are used to calculate structures and properties of glasses.
- Realistic potential are not available for series of NABS glasses as the existing potentials are composition dependent.
- Developing a realistic transferable interatomic potential is crucial to study the structure and properties of boroaluminosilicate glasses.

Introduction

- The goal of this work is to develop useful and transferable force fields for simulating a range of sodium boroaluminosilicate glass systems.
- Molecular dynamics (MD) simulation of multicomponent oxide system like sodium boroaluminosilicate glasses is a complex and challenging problem.
- This potential is based on the sodium borosilicate Potential proposed by Wang et al.. We have added new potential parameters for Al–Al and Al–B to sodium borosilicate potential [3], [4].
- Potential parameters are calibrated against experiment density for a series of sodium boroaluminosilicate glasses.
- MD simulation of multicomponent oxide system like sodium boroaluminosilicate glasses $xAl_2O_3–5B_2O_3 –(80-x)SiO_2 –15Na_2O$ with x = 0, 1, 2.5, 5, 7.5, 10, 12.5, 15, 17.5, and 20 (mol%) [1], [2].
- The difficulty in simulating NABS glasses with Buckingham potential having fixed Partial Charges (e) arises two types of boron atoms that is either three coordinated (B3) or four coordinated (B4).
- The transition from B3 to the B4 happens due to network modifier Na cations acting as charge compensators for B4.
- In the presence of Sodium, B exists in the for coordinated (B4) state. Here, as the (mol%) of Al increases in the system, the sodium rearranges such that it is closer to Al than B because of higher electro-negativity of Al, resulting the conversion of B4 to B3.

Methodology





Initial random configuration

- Initial configurations with 3600 atoms randomly placed with initial density ~2.4 g/cm3.
- MD simulations are carried out using (LAMMPS)[5].
- Time step of 1.0 fs.
- Cut-offs of 11 Å were used for the Buckingham and Coulombic interactions.
- Energy minimization is carried out on these initial random configurations
- The minimized system is then melted at 3000 K in the NPT ensemble
- It is cooled linearly from 3000 K to 300 K in NPT ensemble

Potential parameterization

$$\phi(r_{ij}) = A_{ij}e^{\frac{-r_{ij}}{\rho_{ij}}} - \frac{C_{ij}}{{r_{ij}}^6} + \frac{z_i z_j}{4\pi\epsilon_o r_{ij}}$$

Element	Partial Charge (e)
O	−0.945
Si	1.89
B	1.4175
Na	0.945
Al	1.4175

Bond	A_{ij}(eV)	ρ_{ij}(Å)	C_{ij} (eV.Å6)
Al-B	137.58	0.479	0
Al-Al	351.94	0.521	0
Si-B	337.68	0.290	0
Si-O	50306.36	0.161	46.298
O-Al	28538.41	0.172	34.128
B-B	484.40	0.350	0.000
B-O	206942.87	0.124	35.002
Na-O	120304.42	0.170	0
O-O	9022.84	0.265	85.093

Conclusions

- Using the new potential we simulated all ten glasses with 100 K/ps, 10 K/ps, 1 K/ps and 0.1 K/ps cooling rates.
- Simulated results are compared with experimental data for density, four coordinated boron fraction (B4%) and Elastic properties.
- We show that this new potential can predict structure, density, boron coordination, and elastic properties.
- This empirical interatomic potential exhibits a good transferability to a wide variety of sodium boroaluminosilicate compositions to borosilicate compositions.

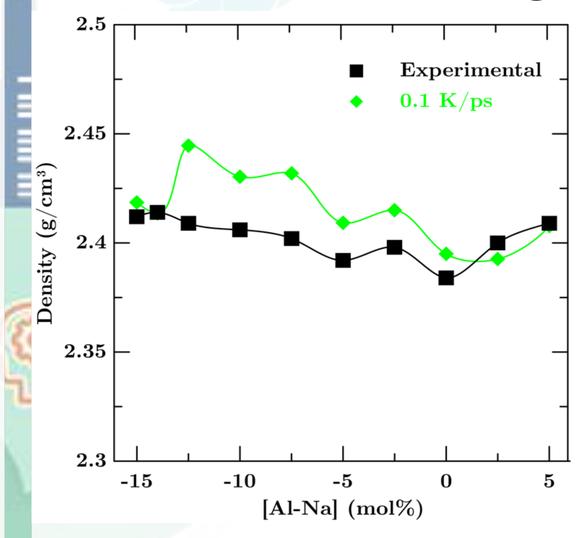
Industrial Significance

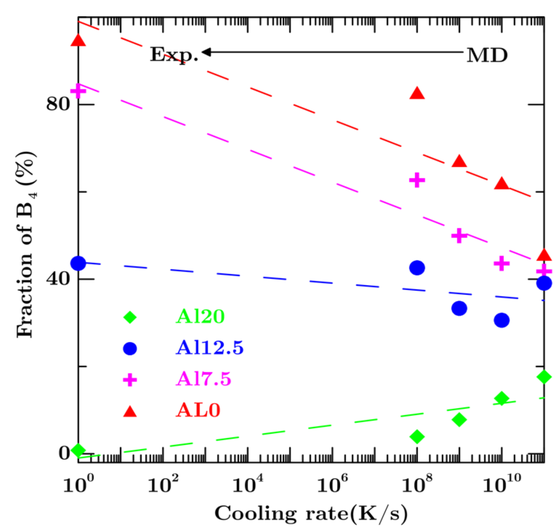
- Reduce product development cycle time of glass manufacturing.
- Bridging the gap between theory and experiments

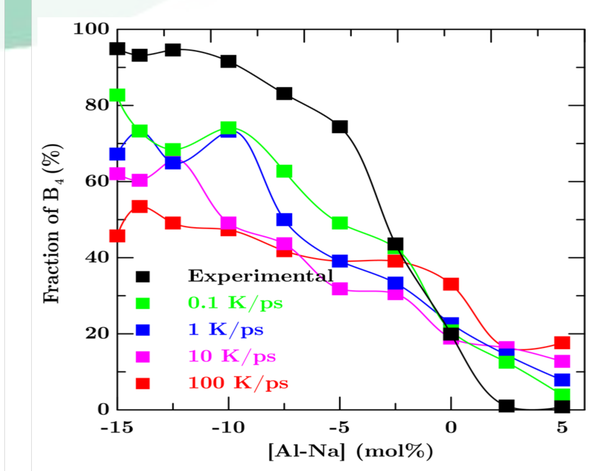
Results

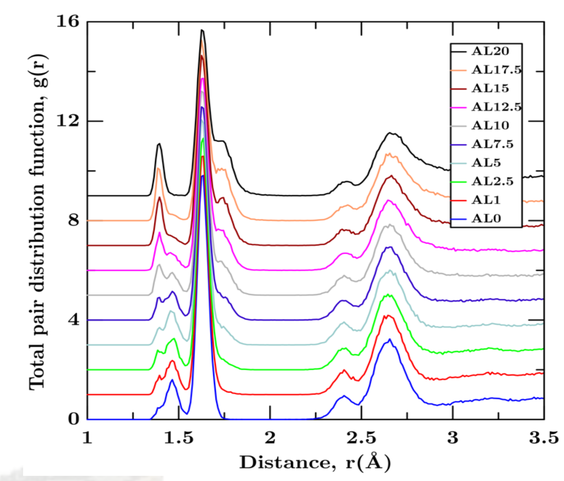
Glass ID	Al_2O_3 (mol%)	SiO_2 (mol%)	B_2O_3 (mol%)	Na_2O (mol%)	Sim. (B4 %)	Exp. (B4 %)	ρ Exp. (g/cm³)	ρ Sim. (g/cm³)
Al0	0.00	80.00	5.00	15.00	82.76	94.90	2.42	2.41
Al1	1.00	79.00	5.00	15.00	73.28	93.20	2.41	2.41
Al2.5	2.50	77.50	5.00	15.00	68.42	94.60	2.44	2.41
Al5	5.00	75.00	5.00	15.00	74.11	91.60	2.43	2.41
Al7.5	7.50	72.60	5.00	15.00	62.73	83.10	2.43	2.40
Al10	10.00	70.00	5.00	15.00	49.09	74.40	2.41	2.39
Al12.5	12.50	67.50	5.00	15.00	42.59	43.60	2.41	2.40
Al15	15.00	65.00	5.00	15.00	20.75	19.90	2.39	2.38
Al17.5	17.50	62.50	5.00	15.00	12.50	1.00	2.39	2.40
Al20	20.00	60.10	5.00	15.00	3.92	0.80	2.41	2.41

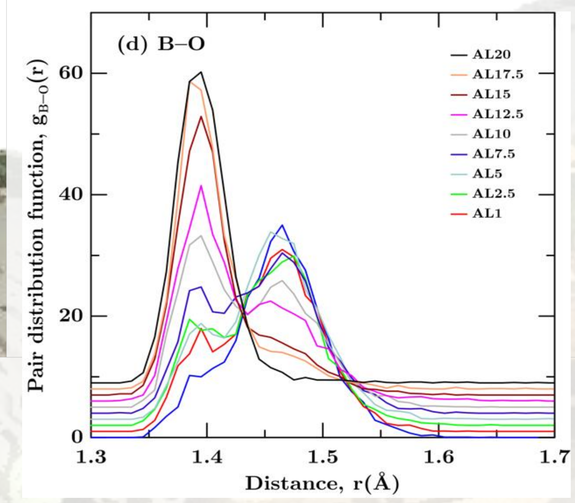
Structure of series of NABS glasses

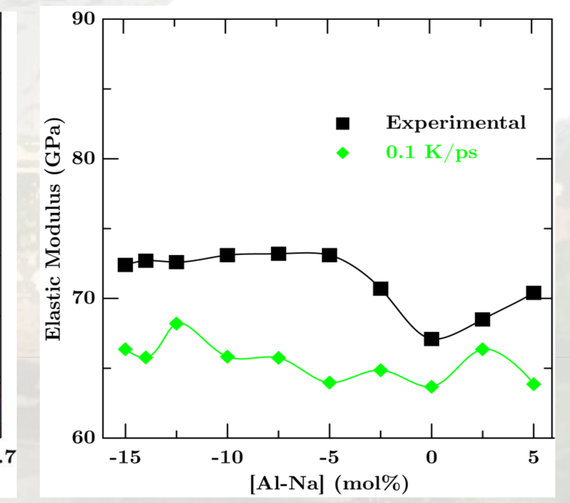












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