Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supporting Information

Molecular Dynamics Simulations of Simplified Sodium Borosilicate Glasses: The Effect of Composition on Structure and Dynamics

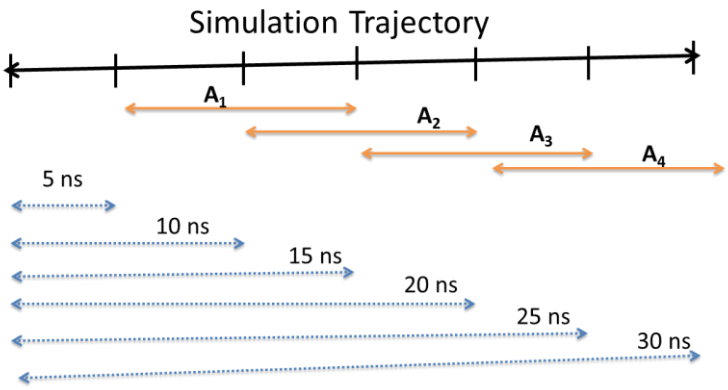
Pooja Sahu[1,2], Sk. Musharaf Ali[*1,2] , K.T. Shenoy[1], Sadhana Mohan[1], A. Arvind[3],

G. Sugilal[2,3], C.P. Kaushik[2,3]

[1]*Chemical Engineering Division, Bhabha Atomic Research Centre, Mumbai, Maharashtra, India*
[2]*Homi Bhabha National Institute, Mumbai, Maharashtra, India*
[3]*Nuclear Recycle Group, Bhabha Atomic Research Centre, Mumbai, Maharashtra, India*

Text S1. Calculation of Average properties and Error Bar

The properties were reproduced from long MD trajectories generated from production run of 30ns simulation length using following method



First, the data points (A_1, A_2, A_3, A_4)were obtained by averaging over 10ns simulation length as shown in image above. Then the average property (A_{avg}) was obtained by

$$A_{avg} = \frac{1}{N}\sum_{i=1}^{N} A_i \qquad \textbf{(s1)}$$

The uncertainties were estimated by standard deviation of data points A_1, A_2, A_3, A_4 using expression shown below

$$\sigma = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(A_{avg} - A_i\right)^2} \qquad \textbf{(s2)}$$

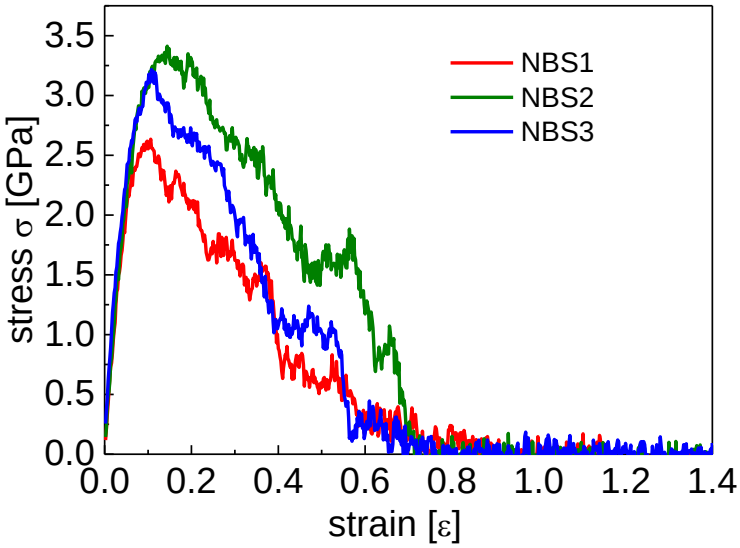


Figure S1: Stress-strain diagram for simulated NBS glasses @ 200K

The elasticity of the simulated glasses was determined via Young Modulus (Y), obtained by slope of line fitted to elastic zone of respective stress-strain curve. In this study, ε=0.01 to 0.04 was used to fit the elastic zone. Young modulus (Y) was measured to be 40.15±1.05, 42.34±1.43, and 39.15±1.06 for NBS1, NBS2 and NBS3 respectively at 200K temperature, which is marginally lower than the measured values at 300K i.e. 40.65±1.94, 42.74±1.72, and 39.66±1.19 respectively for NBS1, NBS2 and NBS3.

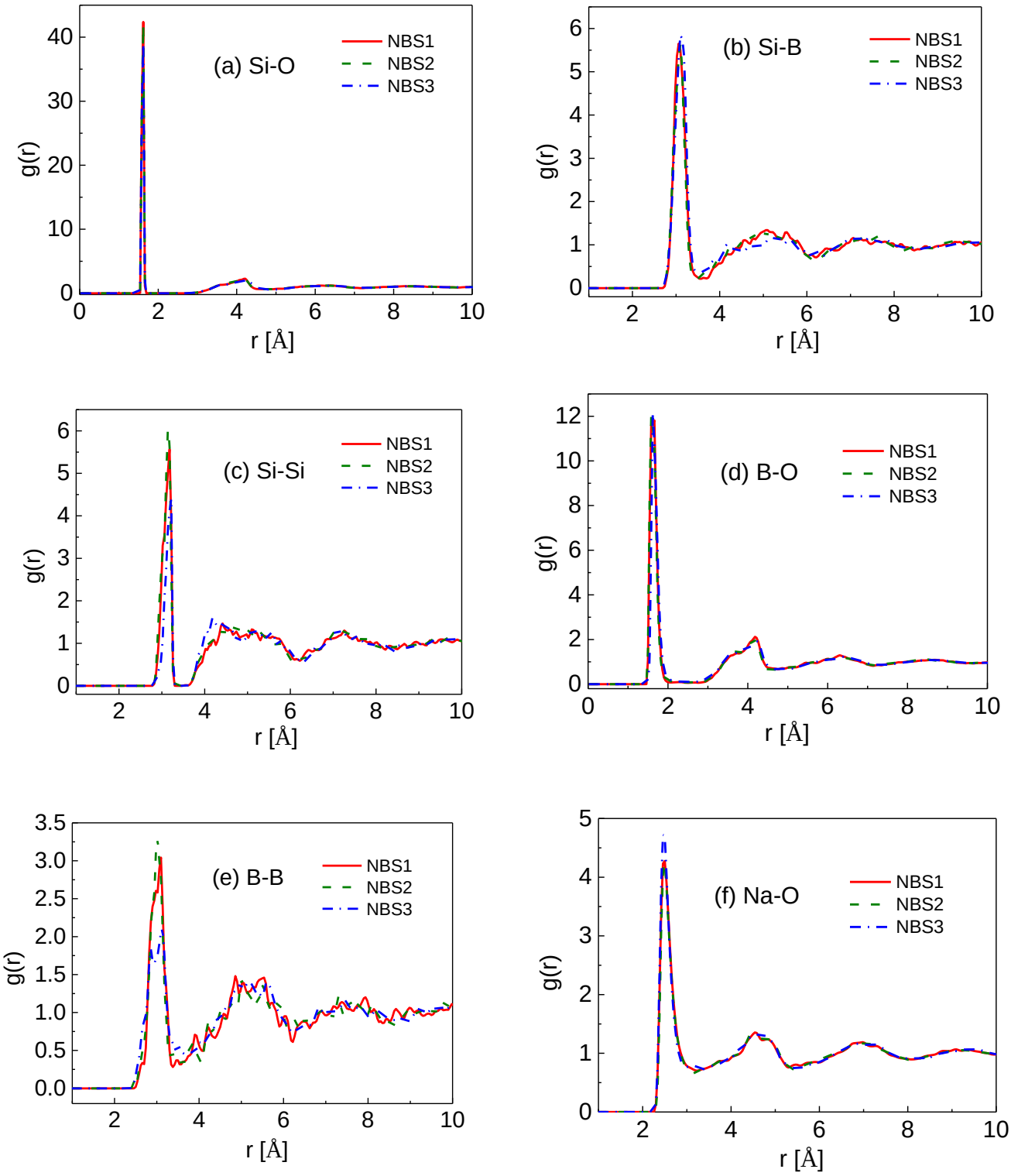
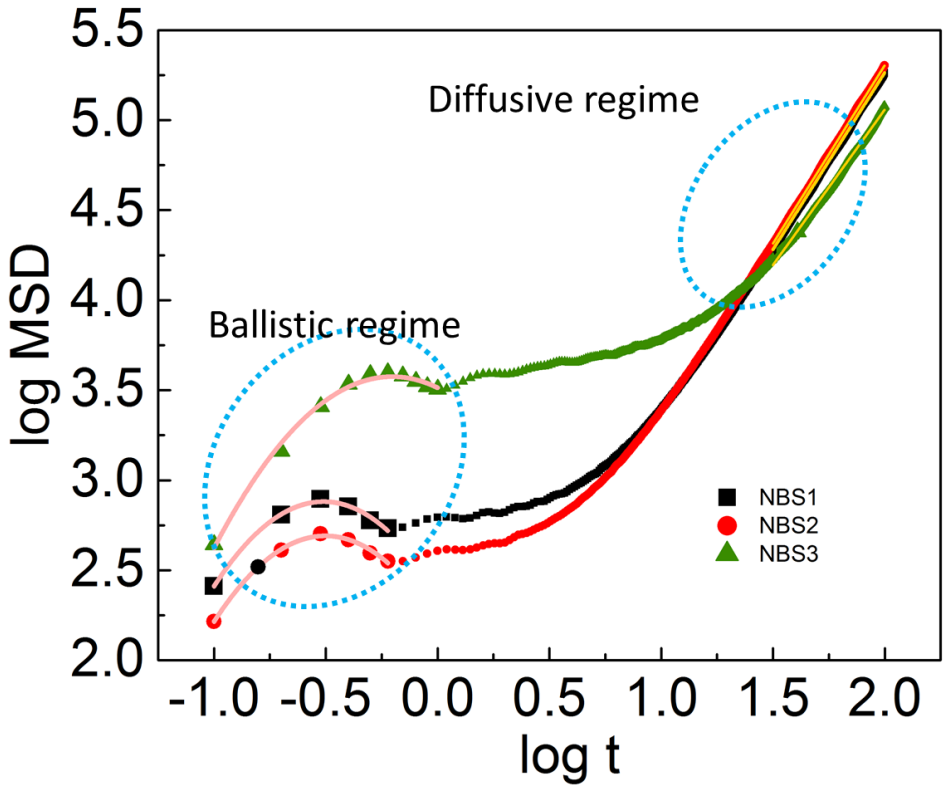


Figure S2: Radial distribution function of pairs (a) Si-O (b) Si-B (c) Si-Si (d) B-O (e) B-B and (f) Na-O for simulated NBS glasses @ 200K



Fitting equations for Ballistic regime

NBS1: $y = 2.37199 - 1.99798x - 1.95913x^2$; $R^2=0.9945$
NBS2: $y = 2.20635 - 1.93149x - 1.92331x^2$; $R^2=0.99613$
NBS3: $y = 3.51371 – 0.60911x - 1.49951x^2$; $R^2=0.99434$

Fitting equations for diffusive regime

NBS1: $y = 1.33063 + 1.96689x$; $R^2=0.99975$
NBS2: $y = 1.34467 + 1.97985x$; $R^2=0.99978$
NBS3: $y = 1.60517 + 1.72668x$; $R^2=0.99775$

Figure S3: log-log plot of MSD vs t for simulated NBS glasses @ 600K

Table S1: RDF peak positions and Coordination number for sodium borosilicate glasses

	NBS1		NBS2		NBS3	
	peak	CN	peak	CN	peak	CN
Si-O	1.58	4.00	1.62	4.00	1.62	4.01
B-O	1.62	3.68	1.58	3.64	1.62	3.57
Na-O	2.50	5.78	2.50	5.65	2.46	6.11
Si-Si	3.18	1.78	3.14	2.04	3.22	1.16
Si-B	3.06	1.95	3.10	1.83	3.10	2.82
B-B	3.10	1.23	3.02	1.25	3.14	1.48