MD calculations for density at high temperature in R_2O-SiO_2 glass melts

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Physical properties of oxide melts are difficult to measure by experiments because of high temperature. Molecular dynamic simulation (MD) is considered a useful method for studying oxide melts and their properties [1-3]. In this work, the compositional and temperature dependence of melt density in R_2O-SiO_2 systems are investigated by utilizing MD simulations with MXDORTO codes developed by Kawamura and development of interatomic interaction model.

Fig. 1 illustrates calculated results of melt density in Na_2O-SiO_2, (a) compositional and (b) temperature dependence. The computed density from 1300K to 1700K using conventional potential parameter, which can reproduce the property at room temperature well, is larger than experimental data. Fig. 2 shows pair correlation functions (PCFs) of Na-O in the computed melt structures. The peak is 2.2 Å that is smaller than the experimental distance of 2.36Å [4] and summation of Shannon ionic radius of 2.35 Å [5]. We consider that the larger density may result from inappropriate distances of R-O using the original potential parameter. By modification of the potential parameter, the agreement with experimental data can be effectively improved. We will elucidate the relationship between the melt structure and the property by analysis by MD using the improved interatomic interaction model.

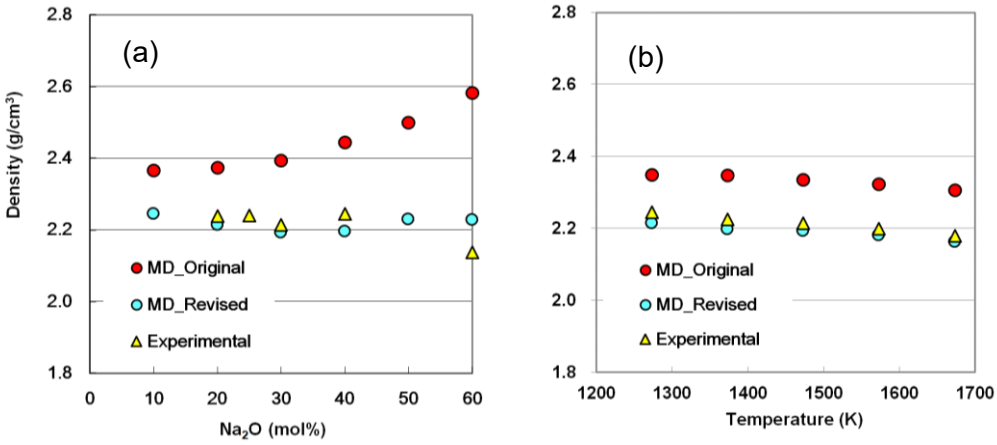

Fig.1 (a) Compositional and (b) temperature dependence of calculated density in Na_2O-SiO_2 compared to experimental data using original and revised potentials.

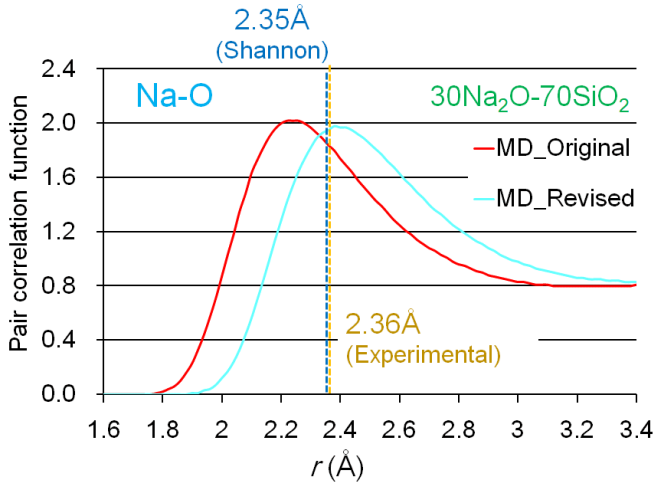

Fig.2 Pair correlation functions (PCFs) of Na-O in $30Na_2O$-$70SiO_2$ with original (red) and revised (light blue) potentials. The orange and blue lines represent the experimental distance [4] and the summation of Shannon ionic radius [5].

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