611a "Caging" Dynamics of a Strong Glass Former

Shi Xu and Janna K. Maranas

[Abstract] By means of molecular dynamics simulation, we study "caging" in dynamics of a strong glass former [boron oxide] by developing a method to calculate the cage size and residence time of each individual atom as it moves from cage to cage. In addition to the average cage size and average first cage escape time, this method provides their distributions. The average cage size and cage size distribution of boron and oxygen atoms are different, resulting from their different extents of connectivity. The cage size distribution shows a short-distance tail resulting from atoms in boroxol rings. Boron and oxygen atoms share the same first cage escape time distribution. A long-time tail is evident in the first cage escape time distribution, again resulting from the rings. The peak in the first cage escape time distribution coincides with the maximum of the non-Gaussian parameter, directly supporting the idea that dynamic heterogeneity is most significant as atoms escape their cages.