Structural origin of fractional Stokes-Einstein relation in glass-forming liquids

Limei Xu, Peking University

In many glass-forming liquids, Fractional Stokes-Einstein relation (SER) is observed after the breakdown of SER above glass transition. As of yet, the origin of such phenomenon remains inclusive. Using molecular dynamics simulations, we investigate the breakdown of SER and the onset of fractional SER in a model of metallic glass-forming liquid. We find that SER breaks down when the size of the largest cluster consisting of trapped atoms starts to increase sharply at which the largest cluster spans half of the simulations box along one direction, and the fractional SER starts to follows when the largest cluster percolates the entire system and forms stable 3-dimentional network structures. Further analysis based on the percolation theory also confirms that percolation occurs at the onset of the fractional SER. Our results directly link the breakdown of the SER with structure inhomogeneity and onset of the fraction SER with percolation of largest clusters, thus provide a possible picture for the breakdown of SER and onset of fractional SER in glass-forming liquids, which is important for the understanding of dynamic properties in glass-forming liquids.

Keywords: Fractional Stokes-Einstein relation, dynamic heterogeneity, structural heterogeneity, metallic glasses

References

1. L. Xu, F. Mallamace, Z. Yan, F. W. Starr, S. V. Buldyrev, H. E. Stanley, Nature Physics 5, 565(2009).
2. S. Pan, Z. Wu, W. Wang, M. Li, L. Xu, (Under Review).