Dynamic Heterogeneity of Ionic and Non-Ionic Drugs Studied Near the Glass Transition by Calorimetric, Dielectric and Mechanical Techniques

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Molecular dynamics of the deeply supercooled liquids is highly heterogeneous. It means that molecules only a few nanometers away from each other may have relaxation rates that differ by several orders of magnitude. Near the glass transition, a significant increase in the length scale of molecular dynamics is observed, which suggests that the spatial heterogeneities can be responsible for the glass transition dynamics [1]. Therefore, in the last half-century, the dynamic heterogeneity of various glass-former liquids has been intensively studied to gain a better insight into our understanding of the glass transition and the related phenomena. The latest theoretical, simulation and experimental investigations suggest that there is a relationship between the glass formation, dynamic heterogeneity, and crystal nucleation, which can play an important role in recrystallization mechanism of amorphous materials [2,3]. One of the most important questions which arises in the heterogeneous picture of molecular dynamics is "how the different molecular interactions affect the degree of the dynamic heterogeneity?". Based on calorimetric, dielectric and mechanical measurements, we evaluate the length scale of heterogeneity for several drugs which are bases (i. e. non-ionic liquids) as well as their hydrochloride salts that belong to protic ionic liquids. Such studies are very interesting, because molecules of these pharmaceuticals have nearly the same chemical structure but their intermolecular interactions are completely different. In this way, we check how the different kinds of intermolecular interactions influence the dynamic heterogeneity of molecular dynamics near the glass transition.

References

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