Density Scaling of Translational and Rotational Molecular Dynamics in a Simple Ellipsoidal Model near the Glass Transition

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For the first time, the single-component ellipsoidal Gay-Berne model has been successfully used to the simulation study of the supercooled liquid state and the glass transition at elevated pressure [1]. Contrary to the single-component Lennard-Jones liquid model, the GB supercooled liquid has turned out to be characterized by the sufficient glass formation ability (Fig. 1) in the thermodynamic range giving the possibility of quite convenient investigations of the translational and rotational molecular dynamics near the glass transition. It seems that this advantage of the GB model over the LJ one originates from the molecular anisotropy inherent in both the ellipsoidal shapes of interacting species and the anisotropic intermolecular potential of the GB model compared to the point interacting species and the isotropic intermolecular potential of the LJ model. One could suspect that the thermodynamic range of supercooling in the GB model might be extended by studying binary mixtures of ellipsoidal species of different α_r, which is worth testing in the future. We have thoroughly explored the density scaling properties in the supercooled liquid state in the anisotropic GB model. We have confirmed the validity of the density scaling of translational (Fig. 2) and rotational relaxation times expressed by some functions and in case of the GB supercooled liquids of four different anisotropy aspect ratios αr, finding that the density scaling exponent γ is the same for τ and τ_{rot} at a given αr and increases with increasing α_r. We have shown that the best way to evaluate the proper value of γ consists in the use of the density scaling criterion, and hence it should be treated as a macroscopic parameter related to the effective short-range intermolecular potential U_{eff} commonly suggested to be composed of a dominant repulsive inverse power law term and a weak attractive background. Our investigations of the supercooled liquid state and the glass transition in the anisotropic GB model clearly show that the anisotropic models constitute a promising alternative to the isotropic ones towards a better understanding and proper reflecting physicochemical properties of the glass forming materials.

REFERENCES

[1] K. Liszka, A. Grzybowski, K. Koperwas, M. Paluch, Density Scaling of Translational and Rotational Molecular Dynamics in a Simple Ellipsoidal Model near the Glass Transition, Int. J. Mol. Sci. 23 (2022) 4546. https://doi.org/10.3390/ijms23094546

FIGURES

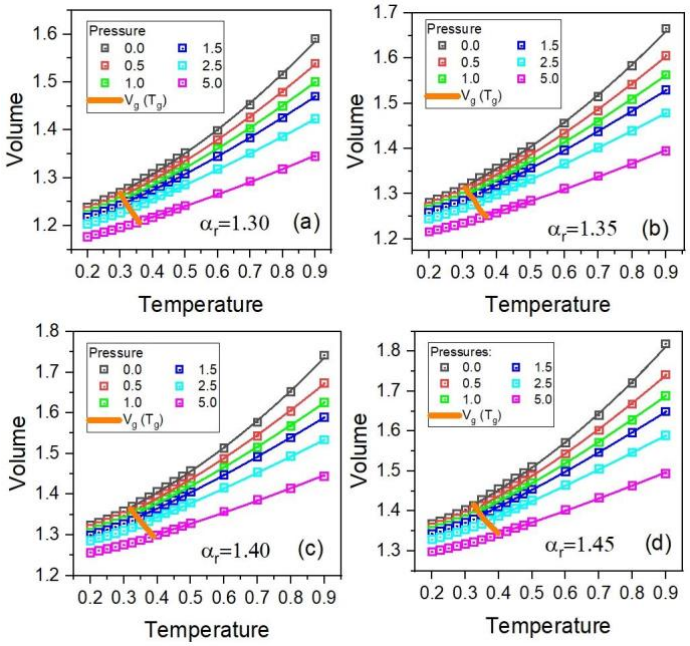

Figure 1: The plots of the isobaric dependences of the particle number volume *V* on temperature *T* in the glassy and supercooled liquids states in the GB model for different anisotropy aspect ratios α_r. The solid curves crossing the isobaric dependences *V* on *T* denote the glass transition curves.

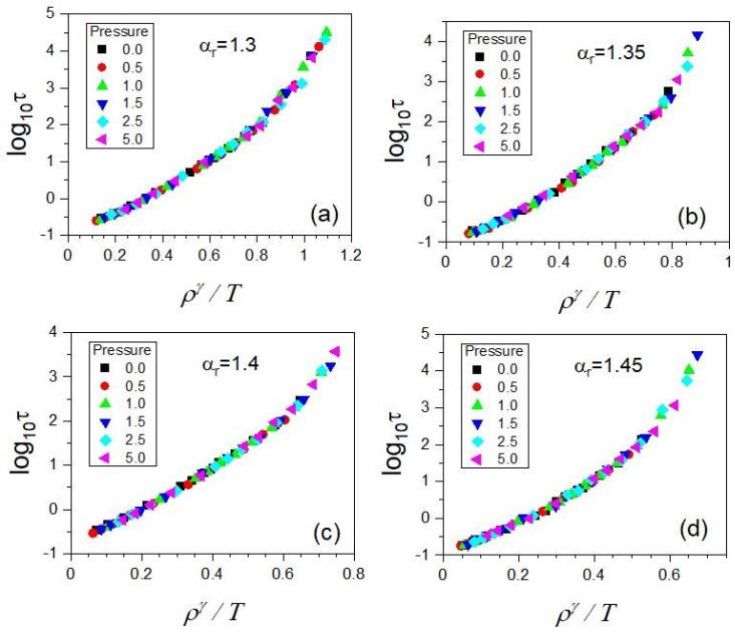

Figure 2: Plots of the high quality density scaling of the translational relaxation times τ collected in the supercooled liquid state in the GB model for different anisotropy aspect ratios α_r, which have been obtained by using the values of the density scaling exponent γ evaluated based on the density scaling criterion.