

A New Class of Equations of State in the Density Scaling Regime

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In the last decade, one of prominent trends [1] in investigating the glass transition and related phenomena has relied on the density scaling law obeyed by molecular dynamics of various materials from different material groups such as supercooled van der Waals liquids, supercooled ionic liquids, polymer melts, and liquid crystals. According to the scaling law, dynamic quantities such as structural relaxation times (or segmental relaxation times in case of polymers), viscosities, and diffusivities can be scaled onto one master curve that is a function of the single scaling variable $(\text{density}^\gamma)/\text{temperature}$ with the scaling exponent γ suggested to be straightforwardly related to the exponent 3γ of the repulsive inverse power law that dominates the effective short range intermolecular potential valid for viscous liquids. Based on the relevant potential, we have derived [2-4] new equations of state (EOSs) in the density scaling regime and very successfully applied them to describe volumetric data of various materials (van der Waals liquids, ionic liquids, polymer melts, and associated liquids) measured in the pressure range $0.1\text{MPa} \leq p \leq 200\text{MPa}$. We have confirmed theoretical grounds for the EOSs by molecular dynamics simulation studies [3,5] and well defined applicability ranges of them and physical meanings of all their parameters. We have shown that the EOSs can be also used beyond the supercooled region. Very recently, we have successfully applied [4] them to investigate a complex, volumetric response of simple liquids measured by the scanning transitiometry.

References

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