

148k Equation of State for Hard-Spheres and Hard-Chains in the Glassy Region

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In this work, we present a theoretically based equation of state that compares well with a recent simulation data of hard spheres in the meta-stable and equilibrium regions. The equation predicts the compressibility factor of hard spheres in the glassy region with an AAD of 2.7% compared with over 10 % for the Speedy [1] equation. The equation was found to accurately represent both the stable and the glassy regions of hard spheres. This is in contrast to available formulations where separate equations are used to represent the stable and glassy regions. Furthermore, this formulation signifies that metastable phase is a continuous extension of stable phase. A mixture version of the equation predicts phase splitting in the glassy region for molecules with large size differences. Equation of state for hard chains valid for the glassy region will also be presented.

[1] Speedy, R. J., "On the Reproducibility of Glasses," J. Chem. Phys., 100, 6684 (1994).