Verification of Thermodynamic Scaling of a nematic phase by a molecular dynamics simulation

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Since thermodynamic parameter Γ in a simple expression of temperature and volume was introduced by McColl, the verification by experiment and simulation has been done. The thermodynamic scaling of liquid crystal phases by dielectric spectroscopy have been studied by Urban and co-workers. Recently, the scaling was extended to the longitudinal relaxation time τ of liquid crystals. The scaling would give important information on a relationship between dynamic property and intermolecular interaction in liquid crystal phase. Here, we study the verification of thermodynamic scaling in the nematic phase by classical molecular dynamics simulation with simple model potentials. In particular, the relationship between thermodynamic scaling and the rotational relaxation time is studied by molecular simulation.

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