Rotational viscosity in liquid crystals: A molecular dynamics study

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Abstract

The molecular dynamics (MD) simulations at various temperatures have been performed for the 4-alkyl-4'-cyanobiphenyls (nCB) with three alkyl groups, pentyl (5CB), heptyl (7CB), and octyl (8CB), in the nematic and isotropic phases. The rotational diffusion coefficient (RDC) was determined by using simulated second and fourth rank order parameters (OPs) and correlation time. The rotational viscosity coefficient (RVC) was computed by the Nemtsov-Zakharov and Fialkowski methods based on statistical mechanical approaches. Temperature and size dependence of the simulated RDC, RVC and OPs has been discussed. Reasonable agreement between the simulated and experimental values was found.