A 2D system of hard needles: event oriented molecular dynamics

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We have simulated the dynamics of a two dimensional system of hard needles by event-oriented molecular dynamics in NEV ensemble. Various quantities namely longitudinal and transverse velocity auto-correlation functions, translational and rotational diffusion mean squared displacements, pressure, intermediate self scattering function, radial distribution function and angular spatial correlation have been obtained and their dependence on number density is characterised. Despite absence of prominent positional ordering, the orientational degree of freedom behaves nontrivially and exhibits interesting features. Slowing down is observed in the angular part of the motion near isotropic-nematic phase transition. It is shown that above a certain number density the rotational mean squared displacement exhibits a three stage temporal regime including a plateau. Comparison to 2D system of hard needles is made and

it is shown that from positional viewpoint, the needle system is more ordered. Many of the temporal autocorrelation functions, both translational and rotational, exhibit a sort of slow dynamics and multi step relaxation. The most interesting feature of the system which has not been explored earlier is the existence of three regimes in the temporal behaviour of the angular mean square displacement. This can be attributed to slow dynamics and possibly the angular glassy dynamics in the system. From the spatial viewpoint, the needle system is less organised than the ellipse system which seems almost structurful. Our findings show that relaxation of the translational degrees of freedom does not smear out angular slow dynamics. The dependence of translational and rotational diffusion coefficients on the number density have been computed and compared to existing results obtained by Monte Carlo simulations.

References

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