ROTATIONAL DIFFUSION AND ORIENTATION OF NANOPARTICLES

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Rotational diffusion processes are correlated with nanoparticle visualization and manipulation techniques, widely used in nanocomposites, nanofluids, bioscience and so on. In the current work, three molecular dynamics (MD) schemes, including two equilibrium (based on MSD relation and autocorrelation function of the angular velocity) and one nonequilibrium methods, are developed to calculate the rotational diffusion coefficient, taking a single rigid carbon nanotube in fluid argon as a case. The three methods produce the same results on the basis of plenty of data with variation of the calculation parameters (tube length, diameter, fluid temperature, density and viscosity), indicative of the validity and accuracy of the MD simulations. However, these results have a non-negligible deviation from the classical literature theory, which is in the framework of continuum-based fluid mechanics and predicts the rotational diffusion coefficient of rodshaped particles. The above deviation may come from some unrevealed factors of the theory at the molecular level, and the adequecy of the theory when applied to pratical situations should be further checked.

When a linear shear flow is imposed to the above system, the single carbon nanotube reveals three forms of anomalous orientation behavior in MD simulations: (i) “Aligned orientation” when the nanotube oscillates around a particular direction which is close to the flow direction at a small angle of about 10° in the velocity-gradient plane; (ii) “Interrupted orientation” when the oscillation is interrupted by a 180° rotation now and then; (iii) “Random orientation” when 180° rotations dominate with the rotational direction coinciding with the local fluid flow direction. The Peclet number serves as an important scaling parameter for processing the results. The orientation order has a positive correlation with the Peclet number, and in turn a negative correlation with the rotational diffusion coefficient, when the diameter of the tube is kept fixed.

Polarizable graphene oxide (GO) particles are prepared by a modified Hummers method, and then they are dispersed in silicone oil to test its electro-responsive thermal properties under imposed DC electric fields. Experiments show a fibrillar structure along the DC electric direction is formed and the structure becomes more ordered with the increase of the electric strength. We further observe that along the oriented direction the thermal conductivity can be enhanced compared to the equilibrium state and the situation can be reversed when the electric fields are removed. At the experimental temperature of 25 ℃ and 50 ℃, the dispersion with a GO mass fraction of about 1% shows a tunable thermal conductivity in the range of 100%~130% below the electric strength of 300 V/mm. In this way, the method of tuning thermal conductivities based on the orientation control of low-dimensional particles is proposed to meet the situation in which a real-time regulation of the thermal properties is required.