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Nanoparticle rotational diffusion and orientation-based thermal smart materials with tunable thermal conductivity

Professor & Deputy dean Bingyang Cao
School of Aerospace Engineering, Tsinghua University

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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 talk, the rotational diffusion is first studied using molecular dynamics since it is closely related to nanoparticle orientation in fluids. 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. 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 rod-shaped particles. When a linear shear flow is imposed to the above system, the single carbon nanotube reveals three forms of anomalous orientation behaviors: (i) “Aligned orientation” when the nanotube oscillates around a particular direction which is close to the flow direction at a small angle of about 10º in the velocity-gradient plane; (ii) “Interrupted orientation” when the oscillation is interrupted by a 180º rotation now and then; (iii) “Random orientation” when 180º rotations dominate with the rotational direction coinciding with the local fluid flow direction. 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. To produce thermal smart materials, polarizable graphene oxide (GO) particles are dispersed in silicone oil to test its electro-responsive thermal properties under imposed DC electric fields. Experiments show a fibrillary 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 room temperature, the dispersion shows a tunable thermal conductivity in the range of 100~200%. 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.

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本件連絡先: 東京大学大学院工学系研究科機械工学専攻 准教授 塩見 淳一郎
GMSIプログラム事務局 E-mail: office@gmsi.t.u-tokyo.ac.jp Phone: 03-5841-0696