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Coarse-grained simulations of flow-induced morphology dynamics in dispersed graphene YUEYI XU, MICAH GREEN, Department of Chemical Engineering, Texas Tech University — We investigated how flow fields affect graphene morphology dynamics in liquid phase using a coarse-grained model. Past simulations of the dynamics of dispersed graphene sheets are limited to static fluids on small timescales, with little attention devoted to flow dynamics, which is critical given the importance of graphene solution-processing of multifunctional devices and materials. We developed a Brownian Dynamics (BD) algorithm to study the morphology of sheetlike macromolecules in dilute solutions with an applied external flow field. We used a bead-rod lattice to represent the mesoscopic conformation of individual two dimensional sheets. We then analyzed the morphology dynamic modes (stretching, tumbling, crumpling) of these molecules as a function of sheet size, Weissenberg number, and bending stiffness. The physical properties (e. g. viscosity) affected by the morphology are also studied. Our results demonstrate how bending stiffness relates to relaxation modes during startup of shear.

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