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Brownian Dynamics Simulations of Dispersed Graphene Sheets

YUEYI XU, MICAH GREEN, Department of Chemical Engineering, Texas Tech University — Past simulations of the dynamics of dispersed graphene sheets are limited to static fluids on small timescales, with little attention devoted to flow dynamics. To address this need, we investigated how flow fields affect graphene morphology dynamics using a coarse-grained model; this relatively untouched area is critical given the importance of graphene solution-processing of multifunctional devices and materials. In particular, we developed a Brownian Dynamics (BD) algorithm to study the morphology of sheetlike macromolecules in dilute, flowing solutions. 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. Our results indicate the model can successfully simulate a range of dynamic modes in a given flow field and yield fundamental insight into the flow processing of graphene sheets.

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