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Brownian Dynamics simulations of dilute graphene solutions under flow YUEYI XU, MICAH GREEN, Department of Chemical Engineering, Texas Tech University — Many graphene-based materials (such as thin conductive films and nanocomposites) are processed in the liquid phase and require the conformation and alignment of graphene in solution to be precisely controlled. However, prior studies of conformation dynamics of sheetlike macromolecules such as graphene have been limited to equilibrium behavior, and there have been no studies of the dynamics of sheetlike macromolecules on flow processing timescales. Here we develop Brownian Dynamics (BD) algorithms in order to quantify the effects of flow processing on graphene conformation. The method is conceptually similar to those used for linear polymers; we coarse-grain the sheet using a bead-rod lattice of arbitrary 2-D connectivity and develop a novel theoretical framework for bending and metric forces. Using this technique, we simulate the conformation dynamics of dilute sheetlike macromolecule solutions in shear flow and compute the corresponding solution properties as a function of flow strength, sheet size, and solvent quality.

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