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Brownian Dynamics Simulation of two-dimensional nanosheets under extensional flow YUEYI XU, Department of Chemical Engineering, Texas Tech University, MICAH GREEN, Department of Chemical Engineering, Texas A&M University — We investigated the morphology change of two-dimensional nanosheets under extensional flow using a coarse-grained model. Nanosheets such as graphene are promising materials for a variety of materials and electronics applications; extensional flow fields are used to cast or process liquid nanosheet dispersions in several processing techniques, including spin coating and compression molding. Process parameters, including bending stiffness and Weissenberg numbers can have a significant impact on the nanosheet morphology and the physical properties of the finished products. We use Brownian Dynamics simulations to study the impact of external flow field on a two-dimensional bead-rod lattice model. Our model was previously demonstrated for steady shear flow. Here we studied the change of morphology of graphene over time and varied the sheet size, bending stiffness and Weissenberg number. Our results showed a flattening behavior that increases with Weissenberg number. Our results also showed significant differences between nanosheets as a function of bending stiffness, with contrasting "plate" and "washrag" results under extension. The intrinsic viscosity first experiences a drop with Weissenberg number followed by a plateau associated with maximum extension.

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