Abstract Submitted
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Shear-induced exfoliation of graphite nanoplatelets into graphene: insights from non-equilibrium molecular dynamics[1] SIMON GRAVELLE[2], CATHERINE KAMAL, LORENZO BOTTO[3], School of Engineering and Materials Science, Queen Mary University of London, E1 4NS, London, UK — Graphite nanoplatelets suspended in a shear flow can be exfoliated into single-layer or few-layers graphene. Such liquid-phase exfoliation method is a promising technique for the production of graphene on large scales, but the micro and nanoscale fluid-structure processes controlling exfoliation are not understood. Here we use molecular dynamics simulations of a defect-free graphite nanoplatelet suspended in a shear flow to characterise the exfoliation dynamics and measure the critical shear rate above which exfoliation occurs, comparing the effect of using different solvents (water and NMP). The measured critical shear rates are compared with a simple theoretical model due to Chen et al. (Chem. Commun., 48. (2012) 3703-3705) based on a balance between the work done by viscous shearing forces and the change in interfacial energies upon layer sliding. We found it difficult to reconcile the molecular dynamics results with the model. The results obtained so far highlight the importance of hydrodynamic slip at the liquid-graphene interface, and the effect of graphene edges on hydrodynamics and interfacial mechanics. Both effects are incompletely included in the model.

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