Compressible Flow Exfoliation of Graphene: A Multiscale Study

Saeed Arabha, Cuiying Jian, Reza Rizvi*
Department of Mechanical Engineering, Lassonde School of Engineering, York University, Toronto ON, Canada
*reza.rizvi@lassonde.yorku.ca

ABSTRACT
The field of two-dimensional (2D) nanomaterials has gained significant interest over the last few decades in numerous applications because of their unique properties that exhibit when a bulk material is reduced to its 2D form. A wide variety of 2D layered materials have been synthesized by a newly developed compressible flow exfoliation (CFE) process, which has considerable advantages over current top-down approaches. In this study, computational fluid dynamics (CFD) and classical molecular dynamics (MD) are used to investigate the interactions of gas particles with pristine, unfunctionalized graphene sheets during the CFE process and try to understand the atomistic mechanism of layer separation. The thermal vibration of graphene layers caused by the elevated temperature of a flowing gas medium can accelerate the exfoliation tendency. However, it is insufficient to overcome the binding energy between graphene layers while the gas particles are static. Therefore, a range of one-directional flow velocities is applied to the compressible fluids based on the experimental findings, and dispersion of graphene is observed when the velocity exceeds the supersonic flow condition. Analyzing the dynamic properties of exfoliation, it is established that sliding in the parallel direction is the preferable exfoliation mechanism of graphene than vertical separation. Furthermore, the upstream pressure plays a fundamental role in controlling the gas density and flow velocities during exfoliation. It is also observed that a heavier gas is less conducive for delaminating graphene than a lighter gas because of its higher atomic mass and lower flow rates at identical conditions. The findings of this study provide more flexibility to synthesize graphene and other 2D materials at a multitude of processing conditions using compressible gases.