Project No. and Title of the Project: GAP-52, Development of Multiscale Framework for Investigating the Role of Carbon-Based Nanomaterials in Enhancing the Component-Level Performance of Offshore Engineering Structures

Funding Body: SERB, Department of Science & Technology (DST), India

This project focused on developing a multiscale computational framework to investigate nanoscale friction and interfacial behaviour in graphene, hexagonal boron nitride (h-BN), and graphene/h-BN heterostructures. Molecular dynamics simulations, and atomistic–continuum coupling approaches were employed to study the influence of loading, temperature, defects, adhesion, and substrate properties on tribological performance.

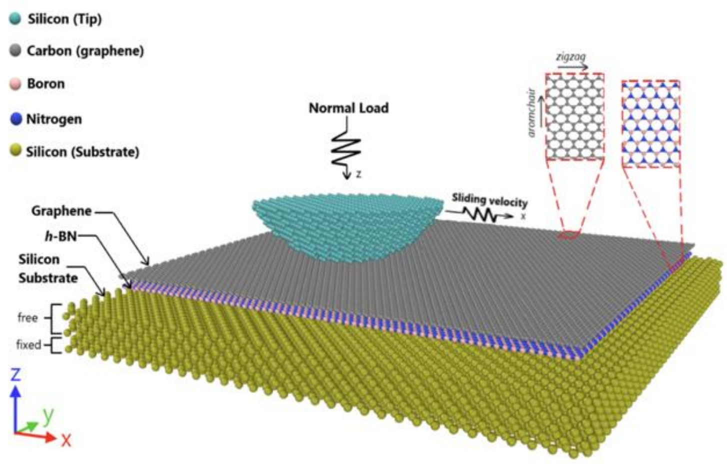

Figure 1: Model for Si tip sliding over graphene/h-BN heterostructure coated over silicon substrate.

Significant Achievements/Outcomes: The project advanced the understanding of nanoscale friction mechanisms in graphene, h-BN, and graphene/h-BN heterostructures. The study demonstrated the strong influence of substrate stiffness, interfacial adhesion, temperature, and stacking sequence on frictional behaviour. Bilayer materials exhibited substantially lower friction than their single-layer counterparts, while h-BN/graphene heterostructures showed superior lubricating performance owing to reduced interfacial adhesion. The research further revealed that Stone–Wales defects and moiré superlattice patterns can be strategically utilised to tailor frictional properties in 2D materials. In addition, a concurrent MD–FE multiscale coupling algorithm was successfully developed and validated, providing a robust platform for future large-scale tribological simulations. The outcomes contribute towards the design of advanced low-friction coatings and solid lubricants for offshore engineering systems, MEMS/NEMS devices, and other high-performance engineering applications.