Investigating the effect of size, shape, and strain on the sliding behavior of bilayer graphene using a continuum-based approach.

Gourav Yadav*†[1], Shakti S. Gupta[1], and Roger A. Sauer[2,3,4]

[1]Indian Institute of Technology [Kanpur] – India
[2]Ruhr University Bochum = Ruhr-Universität Bochum – Germany
[3]Gdańsk University of Technology – Poland
[4]Indian Institute of Technology Guwahati – India

Abstract

Two-dimensional (2D) materials like graphene, hexagonal boron nitride (hBN), and transition metal dichalcogenide (TMD) exhibit exceptional individual properties(**1-2**). However, even more exciting phenomena emerge when similar or dissimilar 2D materials are stacked to form layered crystalline structures. These materials possess significant interfacial properties, along with local and global structural modulations influenced by strain engineering and junction types. These factors govern various critical properties such as superlubricity, superconductivity, directional friction, and interlayer stiffness. These features are crucial for applications in MEMS/NEMS devices, sensors, composites, flexible electronics, and optoelectronics(**3-4**).
The superior properties of stacked 2D materials arise from the coupling of strong intralayer elastic interactions with weak interlayer van der Waals forces. Over the past decade, several studies using molecular dynamics (MD) simulations and density functional theory (DFT) have explored the effects of size, shape, lattice mismatch, and external loading on these materials(**5-6**). While these methods have provided results consistent with experimental findings, there remains a need for theoretical and continuum-based approaches to establish generalized relationships and reduce computational costs.

To address this, we developed a continuum-based numerical model to study the interfacial sliding properties of bilayer graphene. Our model investigates the effects of size, shape, lattice mismatch, and loading conditions on the behavior of these materials. The study highlights surface reconstruction phenomena, which are critical for electronic devices, and identifies directional sliding stiffness with potential applications in sensors. For example, in gas sensors, the van der Waals absorption of gas molecules on the layered structure's surface can alter the interfacial vibrational frequencies of the sheets. Our approach offers a computationally efficient and cost-effective means to understand and predict the behavior of layered 2D materials, paving the way for advancements in various technological applications.

References:

*Speaker
†Corresponding author: Gouravphdm20@iitk.ac.in

1. Lei, Y., Zhang, T., Lin, Y.C., Granzier-Nakajima, T., Bepete, G., Kowalczyk, D.A., Lin, Z., Zhou, D., Schranghamer, T.F., Dodda, A. and Sebastian, A., 2022. Graphene and beyond: recent advances in two-dimensional materials synthesis, properties, and devices. ACS Nanoscience Au, 2(6), pp.450-485.
2. Lin, Y.C., Torsi, R., Younas, R., Hinkle, C.L., Rigosi, A.F., Hill, H.M., Zhang, K., Huang, S., Shuck, C.E., Chen, C. and Lin, Y.H., 2023. Recent advances in 2D material theory, synthesis, properties, and applications. ACS nano, 17(11), pp.9694-9747.
3. Geim, A.K. and Grigorieva, I.V., 2013. Van der Waals heterostructures. Nature, 499(7459), pp.419-425.
4. Novoselov, K.S., Mishchenko, A., Carvalho, A. and Castro Neto, A.H., 2016. 2D materials and van der Waals heterostructures. Science, 353(6298), p.aac9439.
5. Dai, Z., Lu, N., Liechti, K.M. and Huang, R., 2020. Mechanics at the interfaces of 2D materials: Challenges and opportunities. Current Opinion in Solid State and Materials Science, 24(4), p.100837.
6. Wang, J., Khosravi, A., Vanossi, A. and Tosatti, E., 2024. Colloquium: Sliding and pinning in structurally lubric 2D material interfaces. Reviews of Modern Physics, 96(1), p.011002.