Slip divergence of water flow in graphene nanochannels: the role of chirality

Graphene has attracted considerable attention due to its characteristics as a 2D material and its fascinating properties, providing a potential building block for nanofabrication. In nanochannels the solid-liquid interface plays a non-negligible role in determining the fluid dynamics. Therefore, for an optimal design of nanofluidic devices, a comprehensive understanding of the slippage in a water flow confined between graphene walls is important. In nanoconfinement, experimental and computational studies have found the slip length to increase nonlinearly when the shear rate is larger than a critical value. Here, by conducting molecular dynamics simulations, we study the influence of the graphene crystallographic orientation on the slip boundary conditions inside a nanoslit channel. The flow in channels with heights of 2.0, 2.4 and 2.8 nm is driven parallel to the zig-zag and arm-chair crystallographic directions. We extract flow rates, velocity profiles, slip velocities and slip lengths. The slip velocity displays a linear relationship to the shear stress up to a critical value, which is not size dependent. Moreover, the slip length is found to be shear stress dependent above a critical shear stress value of 0.4 MPa. Furthermore, our results indicate that after this critical shear stress is reached, the flow rates are significantly influenced (up to 10%) by the particular orientation of the graphene topology.