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Effect of Underlying Substrate on Interfacial Heat Transfer in Graphene Channels¹ DIEGO BECERRA, Universidad de Concepcion, JENS HONORE WALTHER, Technical University of Denmark, HARVEY A. ZAMBRANO, Universidad Tecnica Federico Santa Maria — Graphene is a 2D monoatomic-thick sheet of carbon atoms with exceptional thermal, electrical and mechanical properties. In addition to these properties, graphene exhibits ultra-low friction to water flow making graphene a promissory material to be used in nanofluidic conduits. Transport of fluids in nanochannels is substantially governed by interfacial phenomena therefore interfacial thermal resistance is an important parameter for the design of efficient nanofluidic devices. In this work, we employ atomistic simulations to study the role of the underlying substrate on interfacial heat transport in graphene channels. In particular, we conduct non-equilibrium molecular dynamics simulations of Poiseuille-like flow of water in pristine graphene channels and in channels with walls consisting of graphene supported on slabs of hexagonal boron nitride, silica and polyamide, respectively. For different imposed pressure gradients, we compute velocity and temperature profiles across the channels. Moreover, in order to analyze the relation between heat transfer and water structuring at the solid-liquid interface, for each graphene channel, we compute water ordering, interfacial viscosity and energy landscapes.

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