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Interfacial thermal transport and phonon-phonon conversion at the graphene-boron nitride lateral interface ZHUN-YONG ONG, GANG ZHANG, YONG-WEI ZHANG, Inst of High Perform Comp — Using the nonequilibrium Green's function method, we compute the the thermal boundary conductance of a monolayer graphene-boron-nitride (Gr-BN) lateral heterostructure with an armchair interface. At 300 K, the thermal conductance of the Gr-BN interface is computed to be 3.5 nW/nm^2 or equivalent to approximately 200 nm of BN. The application of a strain, parallel or normal to the interface, also reduces the interfacial thermal resistance by improving the transmission of acoustic phonons. We do a modal decomposition of the phonon transmission spectrum and identify the phonon scattering channels responsible for heat transfer at the interface. We show that at low frequencies, interfacial heat transfer is dominated by the longitudinal, transverse and flexural acoustic phonons while at higher frequencies, it is mostly by longitudinal acoustic and optical phonons. Our work sheds light on the mechanism of phonon-phonon conversion at the interface of 2D lateral heterostructures and how it can be modified via the application of strain.

[1] Levendorf et al., Nature 488, 627 (2012); Liu et al., Nature Nanotechnology 8, 119 (2013)

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