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Ballistic Thermal Conductance in Layered Two-Dimensional Materials ZUANYI LI, Dept. of Electrical Eng., Stanford Univ.; Dept. of Phys., Univ. of Illinois at Urbana-Champaign, YIZHOU LIU, Dept. of Phys. and State Key Lab of Low-Dimensional Quantum Physics, Tsinghua Univ., YONG XU, Dept. of Phys., Stanford Univ., WENHUI DUAN, Dept. of Phys. and State Key Lab of Low-Dimensional Quantum Physics, Tsinghua Univ., ERIC POP, Dept. of Electrical Eng., Stanford Univ. — The thermal properties of two-dimensional (2D) materials like graphene, h-BN, MoS_2 and WS_2 are uniquely anisotropic, including high in-plane but low out-of-plane thermal conductivity κ. Here we provide a comparative study of the ballistic limits of heat flow in these 2D layers and stacks. Based on full phonon dispersions from density functional theory, we calculate their in-plane and cross-plane ballistic thermal conductance per cross-sectional area, G. For a given material, monolayers and multilayers have similar in-plane G above 100 K, but monolayers show higher G at low temperature due to the contribution of flexural phonons. At 300 K, graphene has the highest $G \sim 4.2$ GWK^{-1}m^{-2}, about 20% higher than h-BN and 5 times higher than MoS_2 and WS_2. Cross-plane values are about one order of magnitude lower than in-plane values due to weak van der Waals interactions. Based on the calculated G, we can obtain phonon mean free path, given diffusive κ. These results are important as they establish the length scales of the ballistic-diffusive transition of heat flow and the non-classical regime where κ depends on the system size.

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