Effect of Twist Angle on Interfacial Thermal Transport in WS_2 Bilayers: A Phonon Engineering Study.

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Two-dimensional (2D) materials are promising candidates for next-generation thermal management devices due to their atomically layered structures, which introduce rotational degrees of freedom. [1,2] Theoretical studies have shown that interfacial and in-plane thermal transport in 2D materials are highly dependent on the twist angle. This dependency arises from the twist angle's ability to modulate interlayer phonon coupling, thereby influencing phonon transmission at the interface and scattering in cross-plane phonon transport. Notably, theoretical calculations show that these effects become most pronounced at small twist angles (0–5°). (see Figure 1, A). [3,4] However, fabricating high-quality small angle twisted bilayers with precise control remains challenging, and there are not yet enough experimental studies to fully validate the predictions of theoretical calculations. In this study, we synthesized high-quality monolayer WS_2 via a capping technique-assisted CVD method and fabricated large-area twisted bilayer WS_2 with different twist angles using a water-assisted transfer process (see Figure 1, B). We investigated their interfacial thermal transport properties by measuring the thermal boundary conductance (TBC) with frequency-domain thermoreflectance (FDTR) and in-plane thermal conductivity using microscopic Raman spectroscopy. To further explore phonon transport mechanisms, we compared experimental findings with molecular dynamics (MD) simulations. This study aims to understand how interlayer coupling influences phonon transport in twisted bilayer WS_2. Small twist angles (0°–5°) are expected to be a critical regime where the interplay between phonon transmission and scattering, governed by interlayer coupling strength, undergoes significant variation. This balance may provide insights into phonon engineering and impact the design of tunable thermal management systems for nanoscale devices.

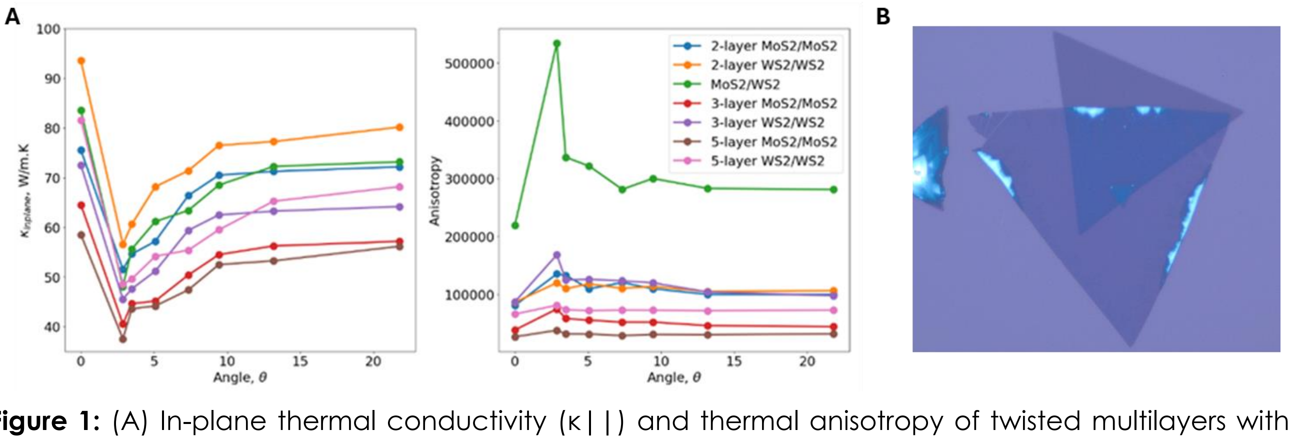

Figure 1: (A) In-plane thermal conductivity (κ||) and thermal anisotropy of twisted multilayers with respect to the applied twist angles. (molecular dynamics simulations on the in-plane and cross-plane thermal conductivity of both homo- and heterogeneous layers of TMDCs). (B) Twisted bilayer with an angle of 23° fabricated in our study.

References
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