

Direct measurements of anisotropic thermal transport in 2D materials and heterostructures

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To effectively realize the potential of two dimensional (2D) materials (2DMs) in heat management, power electronics, new semiconductor processors, and thermoelectric applications, it is essential to measure heat transport in 2DMs and their heterostructures. This task presents several formidable challenges: the measurements are to be done on nanometre-scale thick 2DMs with structures often consisting of flakes of only a few μm across, with multiple interfaces, and with a highly anisotropic nature of heat conductance due to strong covalent bonds in atomic planes vs weak van der Waals (vdW) bound atomic layers. Here we report a pioneering approach for direct measurements of anisotropic thermal conductivity in 2DMs. The approach uses scanning thermal microscopy, SThM, that while sensitive to heat flow to a sample via nanoscale probe tip [1], on its own neither can quantify thermal conductivity due to generally unknown probe-sample thermal resistance nor can detect the anisotropy of the thermal conductivity. We, therefore, combine SThM with the measurements of 2DMs and their heterostructures at variable thickness by using dedicated Ar-ion cross-sectioning [2] to produce a low-angle wedge structure (inset in Fig. 1a). By scanning SThM across such wedge we obtain in a single measurement (Fig 1b,c) heat conductance as a function of thickness. For low thicknesses (compared with the size of the probe-sample contact), the heat transport is predominantly normal to the layers, while at larger thicknesses it becomes three-dimensional, with such transition directly affected by the anisotropy of the thermal conductivity of the 2DM sample. Using a simple analytical Musychka-Spiece model [2], validated by the finite element analysis, we first find the dimensions of the SThM tip-sample thermal contact using the test wedge sample of a known material (e.g. isotropic SiO_2 on Si) via the simple curve fitting (Fig 1d) and then find the absolute in-plane and cross-plane values of thermal conductivities of 2DMs. We use x-SThM for measurements of the γ -InSe nanolayers with in-plane and cross-plane conductivities of $2.16 \text{ Wm}^{-1}\text{K}^{-1}$ and $0.89 \text{ Wm}^{-1}\text{K}^{-1}$, respectively [3], 2DM perovskites for advanced solar cells [2] and superlattices of MoS2 interspersed with nanolayered Sb_2Te_3 [4] where the extremely low in-plane thermal conductivity of $0.7 \pm 0.1 \text{ Wm}^{-1}\text{K}^{-1}$ lead to record values of thermoelectric figure of merit ZT of 2.08 ± 0.37 at room temperature.

References

- [1] Spiece, J. et al J Appl. Phys. 124 (1) (2018) 015101.
- [2] Maiti, A. et al, Phys. Rev. Mater. 7 (2) (2023) 023801
- [3] Gonzalez-Munoz, S. et al, Adv. Mater. Interfaces, (2023) in press.
- [4] Ahmad, M. et al, Adv. Funct. Mater. 32 (49) (2022) 2206384.

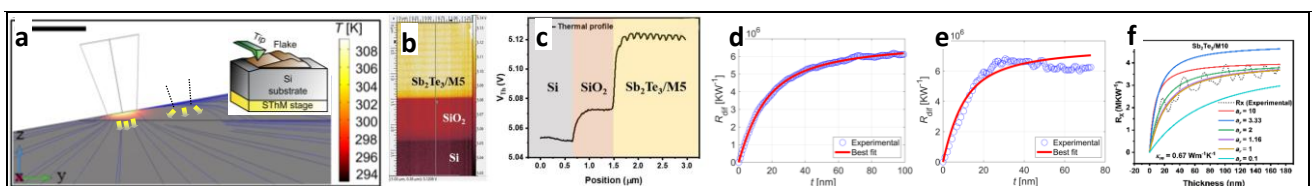


Figure 1: inset in **a)** - Low angle wedge 2D material sample preparation for the cross-sectional SThM. **a)** The finite element analysis modelling of the heat flow for different thicknesses of the 2DM sample on a substrate: the in-plane to cross-plane heat flow ratio changes as the thickness of the sample increases. **b)** x-SThM thermal image of the 2DM $\text{MoS}_2/\text{Sb}_2\text{Te}_3$ superlattice on Si/SiO_2 substrate. **c)** x-SThM thermal response profile across $\text{Si}/\text{SiO}_2/2\text{DM}$ superlattice in b, c). Dependence of thermal resistance vs thickness of the layer for **d)** SiO_2 on Si substrate, **e)** γ -InSe on Si substrate, **f)** $\text{MoS}_2/\text{Sb}_2\text{Te}_3$ superlattice on SiO_2 substrate overlaid with the simulated variable layer anisotropy dependence.