Understanding the in-plane thermal conductivity of $MoSe_2$ from bulk down to the monolayer

D. Saleta Reig[1]
S. Varghese[1], R. Farris[1], J. D. Mehew[1], A. Block[1], O. Hellman[2], P. Wozniak[3], M. Sledzinska[1], A. El Sachat[1], E. Chávez-Ángel[1], S. O. Valenzuela[1,4], N. F. Van Hulst[3,4], P. Ordejón[1], Z. Zanolli[5], C. M. Sotomayor Torres[1,4], M. Verstraete[6], and K. J. Tielrooij[1]
[1] *Catalan Institute of Nanoscience and Nanotechnology (ICN2), BIST and CSIC, Campus UAB, 08193 Bellaterra (Barcelona), Spain*
[2] *Department of Physics, Chemistry and Biology, Linköping University, Sweden*
[3] *ICFO−Institut de Ciències Fotòniques, The Barcelona Institute of Science and Technology, Av. Carl Friedrich Gauss 3, 08860 Castelldefels (Barcelona), Spain*
[4] *ICREA, Pg. Lluís Companys 23, 08010 Barcelona, Spain*
[5] *Chemistry Department and Debye Institute for Nanomaterials Science, Utrecht University, the Netherlands*
[6] *Nanomat, Q-Mat, CESAM, and European Theoretical Spectroscopy Facility, Université de Liège, B-4000 Liège, Belgium*
david.saleta@icn2.cat

Understanding thermal transport in layered materials is crucial for enabling applications in fields like thermal management and thermoelectricity. Furthermore, this understanding is required for properly designing, for example, electronic and optoelectronic devices based on transition metal dichalcogenides (TMDs). However, despite extensive research on the thermal properties of TMDs, there is a lack of studies that systematically vary the flake thickness in the few-layer regime [1, 2, 3] and no consensus exists on how thermal transport changes for different layer thickness.

Recently [4], we have used Raman thermometry to measure the in-plane thermal conductivity of a large batch of suspended $MoSe_2$ flakes with thicknesses ranging from monolayer to bulk. With this technique, we use the calibrated shift of the A_{1g} Raman mode in $MoSe_2$ as a function of temperature, in order to convert power-induced shifts into a local temperature rise per unit absorbed power, which is inversely related to the thermal conductivity of the suspended flake. Besides varying the flake thickness, we study the influence of the environment, heat sinking material, and hole size, in order to identify and eliminate potential experimental artefacts. We obtain thermal conductivity values for few-layer $MoSe_2$ to be in range 15 – 25 W/m/K, weakly influenced by the thickness of the suspended flake. We also find that monolayer flakes are strongly affected by the environment, while thicker flakes are more dependent on proper heat sinking properties.

We complement our experimental findings with state-of-the-art ab-initio simulations that are valid at non-zero temperature. Our simulations show that there are significant changes in the modes that are the main responsible for thermal transport, although these effects subtly cancel each other out, leading to a small thickness effect on the in-plane thermal conductivity. These results may have implications for designing and engineering novel heat-dissipation and related devices.

References

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