SAND2022-8142C

The Influence of Atomic-Scale Defects on Thermal Transport in MoS_2

Pingping Chen, Aroop Behera, Ethan A. Scott, Christopher M. Smyth, Tzu-Ming Lu, Suprem R. Das, and C. Thomas Harris

Transition-metal dichalcogenides, such as molybdenum disulfide (MoS_2), have attracted considerable attention as tunable band-gap semiconductors that may be fabricated in a monolayer format and that give rise to unique electrical and thermal properties. These properties are directly linked to the layer structure, which is sensitive to defects and impurities. While several computational studies have investigated the thermal conductivity of supported and encased MoS_2, the impact of lattice defects on thermal conductivity and thermal boundary conductance in MoS_2 has not been studied experimentally as a function of both defect density and layer number. In this work, we use frequency domain thermal reflectance (FDTR) to study the thermal transport properties of mechanically exfoliated MoS_2 flakes with controlled defect densities and a known number of layers, which are supported on sapphire substrates. The sulfur defect density is controlled via hydrogen-based plasma, and x-ray photoelectron spectroscopy (XPS) is used to characterize the density of these sulfur vacancy defects. In combination with our materials characterization, we provide an effective thermal conductance analysis to explain the reduction in thermal transport due to carrier scattering by vacancies. The results from this study serve to further our understanding of the fundamental physics of phonon transport in the presence of defects and provide a pathway for studying thermal transport in nanoscale electronic devices based upon 2D materials.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.