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Investigating the Thermal Resistance of Individual Grain Boundaries and interfaces Based on Local Thermal Conductivity Imaging

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## Date: Monday, March 18, 2024 15:00-16:00 Venue: Faculty of Engineering Bldg. 2, Room 232

### Abstract:

Grain boundaries (GBs) and interfaces are critical microstructural components that control the performance of electronic and energy materials. GBs segregate impurity atoms, dopants, and lattice strain, and promote the scattering of heat-carrying phonons, profoundly affecting the local and bulk thermal conductivity. While reduced thermal conductivity in bulk polycrystalline materials has been widely reported, there is limited knowledge about the microscopic effects of GBs on heat flow, particularly at micro- and nanoscale distances on the order of the phonon mean free path (MFP) where the impact of GB structure, strain, and chemical composition on the propagation of heat-carrying phonons are expected to be dominant. In this lecture, I will discuss our recent progress in exploring the spatially resolved frequency domain thermoreflectance technique to map the local thermal conductivity at the microscale and around individual random and symmetric GBs in tin telluride (SnTe) and silicon. I will present local thermal conductivity images of large-grained samples selected to isolate the role of GB phonon scattering from grain size effects and other phonon scattering processes that may arise from the sample heterogeneity. I will show that GBs suppress the local thermal conductivity, and the magnitude of the suppression varies with the misorientation angle, roughness and tilt angle of the GB plane, and nano twin segregation, all of which are deduced from electron backscatter diffraction and transmission electron microscopy imaging. I will present a Gibbs excess approach, which we adapted to estimate the GB thermal boundary resistance (TBR) based on the measured local thermal conductivity data. I will also discuss some recent work on encapsulated two-dimensional heterostructures, where we combined FTDR and optothermal Raman spectroscopy to study the size-effects of the thermal conductivity of few layer MoS<sub>2</sub> nanofilms. I will conclude the lecture with some ideas on how GBs and interfaces can be leveraged to tune the thermal conductivity of functional materials.



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### References

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- S. Jiang, D. Lebedev, L. Andrews, J.T. Gish, T.W. Song, M.C. Hersam, and O. Balogun, "Quantitative Characterization of the Anisotropic Thermal Properties of Encapsulated Two-Dimensional MoS<sub>2</sub> Nanofilms. ACS Applied Materials & Interfaces, **15**(7), 10123-10132, (2023)

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