Understanding Thermal Transport from Nanostructured Sources Using Extreme Ultraviolet Measurements, Hydrodynamic Models, and Atomistic Simulations

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Nanostructured materials can exhibit exotic properties and behaviors beyond those accessible in bulk materials, due to the increased influence of surfaces and interfaces. Moreover, at the nanometer length scale, traditional metrology tools struggle to precisely measure the functional properties, and conventional macroscopic models fail to accurately describe the physical phenomena of nanostructured systems. Specifically, the heat flow from nanostructured sources on semiconductor/dielectric substrates—where phonons are the dominant heat carriers—deviates from the traditional Fourier's law of heat diffusion when the length scales of the sources approach those of the relevant phonon mean free paths. While many past experiments and theoretical works explored the breakdown of Fourier's law, there is still no unifying framework for heat transport in arbitrary geometries and no consensus on the fundamental underlying mechanisms. Consequently, this has limited the technological development of functional nano- and quantum-devices, where thermal management often determines the efficiency.

Here, we present new experimental measurements along with both advanced mesoscopic and microscopic models to provide a comprehensive picture of heat dissipation away from periodic 1D-confined (nanoline) and 2D-confined (nanodot) heat source arrays on silicon. Using our ultrafast extreme ultraviolet dynamic scatterometry technique, we show that closely-spaced heat sources cool faster than widely-spaced ones—both for 1D- and 2D-confined sources—which demonstrates that this counterintuitive behavior is present for general geometries. Furthermore, we show that an advanced hydrodynamic transport model accurately predicts the full thermomechanical response of the nanostructured sources for arbitrary geometries. Additionally, we perform atomistic simulations in device-relevant geometries and find results in agreement with both experiments and advanced hydrodynamic predictions. These microscopic simulations access the fundamental phonon dynamics driving the observed behavior, while the mesoscopic model provides a unifying framework for predictive device modeling.