Thermal Conductivity of Nanowires: Machine Learning and Monte Carlo Insights

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The thermal conductivity of nanowires is critically influenced by their structural properties, such as width and surface-roughness parameters (rms roughness, correlation length, and correlation type). Accurate modeling of these dependencies is essential for optimizing nanowire applications in thermal management. In this work, we employ symbolic regression to derive explicit mathematical expressions that capture the thermal transport behavior of silicon nanowires (SiNWs) versus structural properties. By integrating Monte Carlo simulation data with advanced machine learning algorithms, we identify key parameter interactions and quantify their effects on thermal conductivity for temperature at and above 300 K and widths above 20 nm. Our approach offers a bridge between complex numerical models and analytical expressions. This presentation will highlight the methodology, key findings, and implications for both theoretical research and practical applications in thermal transport.

The ultralow measured thermal conductivities in intentionally roughened SiNWs have been reproduced in our phonon Monte Carlo simulations in the diffusive limit with exponentially correlated real-space rough surfaces similar to experimental findings [1,2]. In order to understand the behavior of thermal conductivity with respect to various physical properties of the nanowires, we employed data analysis and machine learning methods to infer mathematical expressions that would relate the termal conductivity to these properties.

Symbolic regression is a machine learning algorithm capable of uncovering analytical equations that describe data, which can result in interpretable models with strong generalization potential beyond the training dataset. In this work, we employ a neural-network-based symbolic regression framework called the Equation Learner (EQL) network [3] and combine it with our Monte Carlo results.

Thermal conductivity values of intentionally roughened silicon nanowires has been reproduced in phonon Monte Carlo simulations with exponentially correlated real-space rough surfaces, and the root mean squared (RMS) surface roughness, correlation length, wire width, temperature, surface area, volume and normalized geometric mean free path (N-GMFP) [1] of the nanowires are saved to be used as the dataset. This dataset was fed to the symbolic regression network in various combinations, and the network was fine tuned to fit the needs of the dataset and be able to produce mathematical expressions that are short and comprehendible. The final symbolic network was formed of two layers, each layer comprising function nodes loaded with identity, square, exponential, sinusoidal and product functions. The variables we fed in the algorithm stayed as variables through the process, and the result was finalized into a partial function of the input variables.

The relation of thermal conductivity with N-GMFP was observed to form compact equations with the two distinct parts of thermal conductivity vs. N-GMFP graph. The results agree with experimental data from literature [2].

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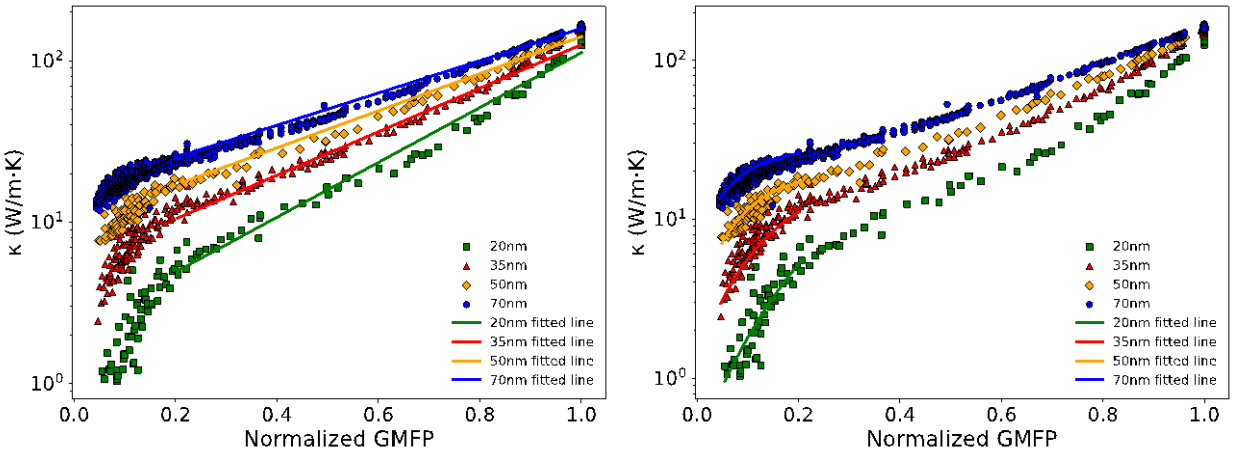

Fig. 1. Thermal conductivity versus normalized geometric mean free path as obtained from phonon Monte Caro simulation (symbols) and from symbolic regression (lines). The left panel highlights the fit for diffusive regime (small to moderate roughness or high normalized GMFP), and the right panel presents the fit for the localization regime (high roughness or low normalized GMFP).

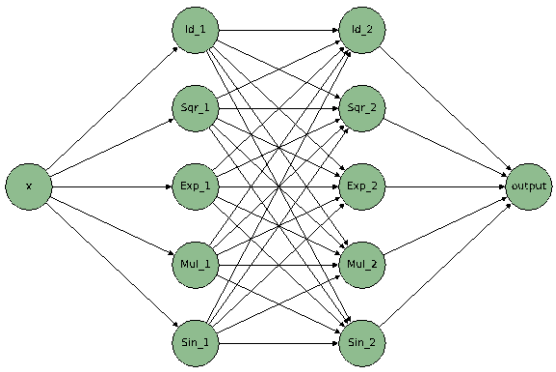

Fig. 2. The equation learner symbolic network schematic. This schematic has two layers of neurons that have identity, square, exponential, multiplication and sinusoidal activation functions in each of the two layers. More nodes with different functions can be added to these layers. [2]