Mechanical Engineering Doctoral Defense

Effects of Advanced Material Morphologies on Thermal, Electrical and Thermoelectric Properties

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Abstract

Progressive miniaturization in electronics demands advanced materials with excellent energy conversion and transport properties. Opportunities exist in novel material morphologies such as hierarchical structures, multi-functional composites and nanoscale architectures which may offer mechanical, thermal and electronic properties tailored to a wide range of applications (e.g., aerospace, robotics, biomedical etc.). However, the manufacturing capabilities have always posed a grand challenge in realizing the advanced material morphologies. Furthermore, the multi-scale modeling of complex material architectures has been extremely challenging owing to the limitations in computation methodologies and lack of understanding in nano-/micro-meter scale physics. To address these challenges, this work considers the morphology effect on carbon nanotube (CNT)-based composites, CNT fibers and thermoelectric (TE) materials. First, we report a computationally efficient two-dimensional (2D) finite element model (FEM) to study the electrical and thermal properties in CNT based composites by simultaneously considering the stochastic CNT distributions, CNT fractions (upto 80%) and interfacial resistances. The FEM allows to estimate the theoretical maximum possible conductivities with corresponding interfacial resistances if the CNT morphologies are carefully controlled, along with appreciable insight into the energy transport physics. Then, we propose a data-driven surrogate model based on convolutional neural networks to rapidly approximate the composite conductivities in a second with accuracy > 98%, compared to FEM taking >100 minutes per simulation. Moreover, this research presents a pseudo 2D FEM to approximate the electrical and thermal properties in CNT fibers at various CNT aspect ratios (up to 10,000) by simultaneously considering CNT-CNT interfacial effects along with the stochastic distribution of inter-bundle voids. The FEM provides the current and heat flow visualization to understand the influence of void distribution and morphology control in CNT bundles. Next, this work reports additively manufacturable TE morphologies and analyze the thermo-electric transport behavior. This work introduces innovative honeycomb TE architectures that showed ~26% efficiency increase and ~25% density reduction compared to conventional rectangular TE architectures. Finally, we report 3D printable compositionally segmented TE architectures which provide record-high efficiencies (up to 8.7%) over wide temperature ranges if the composition and aspect ratio of multiple TE materials are optimized within a single TE device.

March 17, 2023; 1 PM; ERC 490;

Zoom Link: https://asu.zoom.us/j/81505365306