**The Summer Undergraduate Research Fellowship (SURF) Symposium**
**7 August 2014**
**Purdue University, West Lafayette, Indiana, USA**

# Thermo-Mechanical Modeling of Carbon Nanotube Thermal Interfaces

Yide Wang, Sridhar Sadasivam, Timothy S. Fisher
Department of Mechanical Engineering, Purdue University

## ABSTRACT

In the last decade, much research has attempted to develop a highly conducting and mechanically reliable thermal interface material. Vertically aligned carbon nanotube arrays (CNTs) is a promising thermal interface material due to the high thermal conductivity of each CNT and the mechanical compliance of CNT arrays [1].

The computational modeling of CNTs is usually at an atomistic scale; however, atomistic simulations are computationally expensive for modeling macroscopic CNT arrays used in experiments. Coarse grain simulation techniques [2] have been developed to reduce the number of degrees of freedom and hence making large scale simulations computationally tractable. The purpose of this project is to build a nanoHUB tool for performing coarse grain simulations of vertically aligned CNT arrays. The tool simplifies the simulation process and allows for parametric studies that would help in the design optimization of CNT thermal interface materials. Geometric parameters such as CNT array height, spacing, and CNT diameter can be input from the GUI and results such as stress-strain curve and Young's modulus of the array can be downloaded. The pressure dependence of thermal contact resistance can also be obtained from the tool. This tool is expected to be useful to experimental researchers working in the field of CNT-based thermal interfaces.

## KEYWORDS

Carbon Nanotube Arrays, Mechanical Performance, Thermal Contact Resistance.

## REFERENCES

[1] J. Xu and T. Fisher, "Enhancement of Thermal Interface Materials with Carbon Nanotube Arrays," *International Journal of Heat and Mass Transfer,* vol. 49, p. 1658, 2006.

[2] M. J. Buehler, "Mesoscale modeling of mechanics of carbon nanotubes: Self-assembly, self-folding, and fracture," *Materials Research Society,* vol. 21, no. 11, pp. 2855-2856, 2006.