# Relationship of Electrical, Thermal, and Mechanical Properties in Progressively Doped SiC via Chemical Vapor Deposited and Neutron Transmutation Doping

**PI**: J. Rory Kennedy - Idaho National Laboratory

**Program**: NSUF

**Collaborators**: Krzysztof Gofryk, David Hurley, Tsvetoslav Pavlov, Malwina Wilding, Fei Teng, Michael Heighes, Brian Newell, Mukesh Bachhav, Linu Malakkai - INL, Yaqiao Wu – Boise State University

**ABSTRACT:**

This project aims to systematically determine the inherent extrinsic electronic, thermal, and mechanical properties of the semiconductor silicon carbide (SiC) doped with nitrogen via chemical vapor deposition (CVD) and phosphorus via neutron transmutation doping (NTD). The goal is to increase the electrical conductivity of SiC through n-type doping via as-fabricated pre-irradiation and in-reactor NTD and test the **hypothesis** that this increase in the electrical transport will lead to an increase in the electronic contribution to the thermal conductivity. Coupled with the inherent semiconductor property of increasing electrical conductivity with increasing temperatures, an increase in the total thermal conductivity of the material and potentially improved mechanical properties at elevated temperatures will be observed.

SiC has long been advocated for use in advanced reactor designs and components for existing reactors due to its superior properties, including low activation, chemical inertness, radiation stability, and very high temperature performance. SiC is currently used as an advanced fuel component in TRISO fuel kernels and it has been suggested for use in inert matrix fuel and as cladding material as well as in other in-vessel structural components. If the doped SiC, whether through CVD or NTD, can achieve higher thermal conductivity and improved mechanical properties, the study's results will be highly significant. It could revolutionize the use of SiC in in-core component structural materials and provide a major advancement for SiC based cladding materials, where enhanced thermal conductivity is highly desirable. It could also position doped SiC as a potential substitute for the SiC component in TRISO fuels.

The project plan involves determining various relevant properties and characteristics of the doped SiC, focusing on their level of doping, temperature dependence, and the influence of the doping type (CVD vs NTD) and doping element (N or P). The studies are divided into three parts: 1) doping predominantly from pre-irradiation nitrogen doping, 2) a combination of significant amounts of pre-irradiation nitrogen doping and NTD phosphorus doping, which results in the highest levels of doping, and 3) doping primarily from NTD phosphorus doping. From these studies, a comprehensive understanding of how to optimize the performance of doped SiC can be realized. The highest doped materials will be tested first to validate the hypothesis. Following this, lower doped materials will be tested to build the relationships between doping levels, increasing thermal conductivity transition temperatures, type of doping, and element doping.

**Thermal conductivity** up to 1500°C will be determined by measurements of thermal diffusivity (laser flash method), heat capacity, density, and dilatometry. Low temperature (5-300 K) thermal conductivity measurements will be performed using a Quantum Design PPMS apparatus. **Electrical conductivity** measurements will be performed using a four-point probe technique with furnace (high T) or in the PPMS system (low T) as will **Hall effect and Seebeck coefficient** determinations. **Mechanical properties** will be assessed with an Instron load frame (tensile), nano- and micro-indentation apparatus (hardness), laser resonance ultrasound spectroscopy (elastic), and cantilever method (fracture toughness). Methods to address the impurity or **doping levels, electronic structure, and bonding** include photoluminescence and Raman spectroscopies as well as theoretical calculations. When appropriate, **crystal structure** study will be performed via X-ray diffraction and **microstructure** characterizations using electron microscopy and atom probe tomography.

A positive outcome from the project will deliver a demonstration that thermal conductivity increases under doping and higher temperature conditions. Annual reports and publications will deliver quantified relationships between doping level and transition temperatures to increasing thermal conductivity as well as the quantified amounts of thermal conductivity increase at temperature.