NUCLEAR ENERGY RESEARCH INITIATIVE

Implications of Graphite Radiation Damage on the Neutronic, Operational, and Safety Aspects of Very High Temperature Reactors

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Project Description

This project entails experimental and computational investigations to study the radiation effects of graphite in Very High Temperature Reactors (VHTR). Researchers will use molecular dynamic and *ab-initio* molecular static calculations to 1) simulate radiation damage in graphite under various irradiation and temperature conditions, 2) generate the thermal neutron scattering cross sections for damaged graphite, and 3) examine the resulting microstructure to identify damage formations that may produce the Wigner effect.

In both the prismatic and pebble bed VHTR designs, the graphite moderator is expected to reach exposure levels of 10^{21} to 10^{22} n/cm^2 over the lifetime of the reactor, resulting in damage to the graphite structure. Studies of irradiated graphite show changes in the thermal conductivity and heat capacity at fluences less than 10^{21} n/cm^2. These properties depend on the behavior of atomic vibrations (phonons) in the graphite solid. Therefore, it can be expected that any alterations in phonon behavior that would produce changes in these properties would impact thermal neutron scattering, with implications for the neutronic and safety behavior of the VHTR. Another important phenomenon pertains to published data showing that a high-temperature (>1,200°C) Wigner-like effect may exist in graphite. If confirmed, this effect would have direct implications on the safety behavior of VHTRs.

Workscope

The primary objectives will be accomplished through the following tasks:

- Simulate atomic collision cascades in graphite
- Model a perfect graphite supercell, initiate damage cascades using the calculated spectrum, and evolve it using Monte-Carlo techniques
- Calculate dispersion relations and obtain vibrational (phonon) frequency distribution
- Calculate thermal neutron scattering cross sections of imperfect graphite
- Determine stored energy of irradiated graphite samples using differential annealing measurements and compare to simulated values
- Assess phonon density states
- Perform structure studies, comparing irradiated and unirradiated graphite samples
- Use analysis codes to assess the neutronic, operational, and safety aspects of the VHTR