
Phase Equilibria and Thermochemistry of Advanced Fuels: Modeling Burnup Behavior

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ABSTRACT:

Achieving the goal of developing advanced fuel concepts that meet the DOE objectives of being robust, demonstrating high performance, and are more tolerant of accident conditions than current fuel systems will require a thorough understanding of the thermophysical and thermochemical properties of the constituent materials. Non-oxide fuel systems are being explored under the Advanced Fuels Program that hold significant promise for improved performance and accident tolerance, including systems considered in the current proposal: Uranium silicides and uranium mononitride with minor second phase silicide.

Prospective cladding materials currently considered that contribute to improved accident tolerance include silicon carbide composites and ferritic alloys (Fe-Cr-Al base compositions). Thus the proposed effort will develop thermochemical models and values, supported with targeted experiments, to evaluate the various fuel-cladding systems. Such a detailed understanding will serve to aid in relatively early screening of candidate systems to avoid wasted effort, guide development of new fuel forms, and to provide a basis for predicting and modeling fuel performance.

Major deliverables for the project include: Thermochemical assessment and models of phases in the U-Si and U-Si-N systems; thermochemical evaluation supported by experimental measurements of fuel-cladding interactions of nitride, silicide, and composite fuel with baseline zirconium, ceramic composite, and ferritic alloy clads; thermochemical assessment and models of phases supported by experimental measurements for nitride/silicide fuels with key fission products provided in a dataset and reported in refereed publications; at least two graduate students and a post-doctoral fellow will be trained and will publish dissertations and papers.

The deliverables are supported by a set of tasks that include thermochemical modeling of the U-Si, and U-Si-N systems; development of relevant thermodynamic data; preparing and analyzing fuel material samples for input information for the modeling efforts; modeling fuel-cladding interactions with experimental support from compatibility testing; developing models of key fuel-fission product compositions and resultant thermodynamic data together with experimental simulation of fuel-fission product compound formation.

The proposed effort is highly relevant to the objectives of the Advanced Fuels Program for high performance and accident tolerant LWR fuels. The success of nitride- and silicide-based fuel systems is dependent on understanding phase equilibria and thermochemistry of critical compositions in the systems. In addition, the developed data can be used in fuel performance codes to predict in-reactor fuel behavior. Finally, the results of the modeling efforts will also support interpretation of the scheduled irradiation experiments for advanced fuels exploring in-reactor behavior and interactions with cladding materials.