THERMODYNAMIC OPTIMIZATION OF THE UN-PuN-Fe SYSTEM

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Operational safety is the foremost criterion in the design of nuclear power plants (NPPs). Modern NPPs employ a defense-in-depth strategy aimed at preventing the release of radioactive material into the environment. An indispensable step in the safety assessment of any NPP is the simulation of accident scenarios, including severe accident sequences involving core meltdown, and the development of measures for managing and mitigating the consequences of hypothetical severe accidents. Knowledge of high-temperature material properties and phase equilibria among the constituent phases plays a central role in the modelling and prediction of severe accident scenarios in nuclear reactors.

The challenge of incorporating plutonium and minor actinides into the nuclear fuel cycle requires the advancement of fast neutron reactor technology. Alongside sodium-cooled fast reactor technology (BN-800, BN-1200M), lead-cooled fast reactor technology is currently under active development. The Russian BREST-OD-300 reactor project employs a lead coolant, with steel as the fuel cladding material. A novel materials engineering solution is the use of mixed uranium–plutonium nitride (MNUP) as the fuel. Compared with conventional oxide fuel, nitride fuel offers several advantages, including higher density and thermal conductivity. A drawback of nitride fuel is its thermochemical instability at elevated temperatures, which complicates the investigation of its high-temperature properties.

To address the scarcity of thermodynamic data on the high-temperature thermodynamic properties of UN and PuN, the high-temperature heat capacities of these nitrides were modelled on the basis of defect formation contributions and correlations with the properties of uranium and plutonium oxides and carbides. The properties of the nitrides in the liquid state were modelled by exploiting the relationship between heat capacities and coefficients of thermal expansion. The resulting data enabled the calculation of phase equilibria in the quasi-binary UN-PuN system, and its phase diagram was constructed for the first time. Using experimental melting data, the phase diagram of the UN-Fe system was calculated, and the model was subsequently extended to the PuN-Fe system. On the basis of the binary subsystem models, the phase diagram of the ternary UN-PuN-Fe system was calculated. The present work demonstrates that phase equilibria in the UN-PuN-Fe system play a key role in analyzing the thermochemical stability limits of nitride fuel pins with steel cladding.