Materials Science & Engineering Doctoral Defense

Microstructurally Explicit Simulation of Multiphysics Transport Behaviors in Uranium Dioxide

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abstract

Fission products in nuclear fuels pellets can affect fuel performance as they change the fuel chemistry and structure. The behavior of the fission products and their release mechanisms are important to the operation of a power reactor. Research has shown that fission product release can occur through grain boundary (GB) at low burnups. Early fission gas release models, which assumed spherical grains with no effect of GB diffusion, did not capture the early stage of the release behavior well. In order to understand the phenomenon at low burnup and how it leads to the later release mechanism, a microstructurally explicit model is needed. This dissertation conducted finite element simulations of the transport behavior using 3-D microstructurally explicit models. It looks into the effects of GB character, with emphases on conditions that can lead to enhanced effective diffusion. Moreover, the relationship between temperature and fission product transport is coupled to reflect the high temperature environment.

The modeling work began with 3-D microstructure reconstruction for three uranium oxide samples with different oxygen stoichiometry: $UO_{2.00}$ $UO_{2.06}$ and $UO_{2.14}$. The 3-D models were created based on the real microstructure of depleted UO2 samples characterized by Electron Backscattering Diffraction (EBSD) combined with serial sectioning. Mathematical equations on fission gas diffusion and heat conduction were studied and derived to simulate the fission gas transport under GB effect. Verification models showed that 2-D elements can be used to model GBs to reduce the number of elements. The effect of each variable, including fuel stoichiometry, temperature, GB diffusion, triple junction diffusion and GB thermal resistance, is verified, and they are coupled in multi-physics simulations to study the transport of fission gas at different radial location of a fuel pellet. It was demonstrated that the microstructural model can be used to incorporate the effect of different physics to study fission gas transport. The results suggested that the GB effect is the most significant at the edge of fuel pellet where the temperature is the lowest. In the high temperature region, the increase in bulk diffusivity due to excess oxygen diminished the effect of GB diffusion.

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