**Molecular Dynamics and Phase Field Studies of Anisotropy in Grain Boundary Energy and Mobility in UO2**

1,2Jarin French, 1Xianming Bai, 2Yipeng Gao

1*Virginia Tech*, 2*Idaho National Laboratory*

The primary fuel in light water reactors is uranium dioxide (UO2). While in reactor, the fuel undergoes significant microstructural changes (via e.g. grain growth) that impacts fuel performance properties (e.g. thermal conductivity, fission gas release, etc.). Molecular dynamics simulation and phase field simulation methods were used to examine the effect that anisotropy in grain boundary (GB) properties has on microstructural evolution. Molecular dynamics simulations were performed to study the misorientation- and rotation-axis-dependent anisotropy of GB energy and GB mobility in UO2. The results show that there is significant anisotropy in GB mobility, but that GB energy is not strongly anisotropic with respect to these GB characters. The GBs with a rotation axis of <111> are found to have higher mobility in general. Phase field simulations qualitatively examined the impact of anisotropic mobility on grain growth. Preliminary results indicate that anisotropic GB mobility can change the GB migration and grain growth behavior.