

## MATERIALS ENGINEERING SEMINAR

### “Defect Clustering in Irradiated Thorium Dioxide and $\alpha$ -Uranium”

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**Purdue MSE Ph.D. Final Exam**

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#### ABSTRACT

Thorium dioxide (ThO<sub>2</sub>) and metallic uranium ( $\alpha$ -U) represent important alternative nuclear fuels. Investigating the behavior of defects introduced into these materials in an irradiation environment is critical for understanding microstructure evolution and property changes. The objective of this dissertation is to investigate the clustering of point defects in ThO<sub>2</sub> and  $\alpha$ -U under irradiation, into voids and prismatic dislocation loops as a function of irradiation dose rate and temperature. To achieve this, we have developed a mean-field cluster dynamics (CD) model based on reaction rate theory to predict the evolution of self-interstitial atom (SIA) and vacancy loops in neutron-irradiated  $\alpha$ -U. Detailed atomistic simulations have been carried out using molecular dynamics (MD) to study the configuration of such loops and compute their energetics, which are essential parameters of the CD model. Bond-boost hyper-MD simulations have been performed to compute the diffusivity of uranium SIA and vacancies, which govern the kinetics of the clustering phenomenon. Another CD model has been demonstrated for proton-irradiated ThO<sub>2</sub>, considering the clustering of Th and O SIA and vacancies into SIA loops and voids, respectively, with varying sizes and stoichiometry. The compositions of all SIA loops and voids dictated by crystallography of ThO<sub>2</sub> in its fluorite structure have been presented in their respective cluster composition space (CCS). The CD model solves the density evolution of off-stoichiometric loops and voids, with irradiation, in their respective CCS. MD simulations have been performed to compute the energetics of different clusters in their CCS, as parameters of the CD model. Temperature-accelerated MD simulations have been performed to compute the diffusivity of Th and O point defects, that dictates the kinetics of defect clustering on irradiation. In  $\alpha$ -U, the CD predictions show an accumulation of small sized vacancy loops and the growth of SIA loops with irradiation dose, which closely fits the reported size distribution of loops in neutron-irradiated  $\alpha$ -U by Hudson and coworkers. The CD predicted density of defect clusters in proton-irradiated ThO<sub>2</sub>, shows the evolution of near-stoichiometric SIA loops in their CCS. The size distribution of SIA loops at high irradiation doses closely corresponds to the transmission electron microscopy (TEM) observations reported in the literature. Also, the CD model did not predict the growth of voids and vacancy clusters, which is consistent with findings in literature. The model was further used to predict the density of sub-nanometric defect clusters and point defects, on low-dose irradiation, that significantly impairs the thermal conductivity of ThO<sub>2</sub>. An extensive TEM and CD investigation has also been carried out to study the growth and coarsening of SIA loop and voids during post-irradiation isochronal annealing of ThO<sub>2</sub> at high temperatures.

**Date: Monday, June 26, 2023**

**Time: 9:00 A.M.**

**Place: ARMS 1021 or via Webex: <https://purdue.webex.com/join/aelazab>**



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