Atomistic Model of Fission Gas Bubble Re-solution Rate in UO_2

W. Setyawan[1*], M. W. D. Cooper[2], K. J. Roche[1], B. P. Uberuaga[2], D. A. Andersson[2], B. D. Wirth[3], R. J. Kurtz[1]

[1]Pacific Northwest National Laboratory, Richland, WA, USA
[2]Los Alamos National Laboratory, Los Alamos, NM, USA
[3]University of Tennessee, Knoxville, TN, USA
[*]Presenting author: wahyu.setyawan@pnnl.gov

Understanding fission gas release in nuclear fuels requires knowledge of gas bubble distribution. Phenomena that affect bubble distribution include, but not limited to, bubble growth by absorption of gas atoms, bubble coalescence, and re-introduction of gas atoms from the bubble back into the fuel matrix (a process known as bubble re-solution). The driving force for bubble re-solution is mostly due to irradiation damage caused by highly energetic fission products (FPs). In UO_2 nuclear fuels, fission of U-235 yields FPs with a kinetic energy of approximately 60 to 100 MeV. As FPs slow down, their kinetic energy is dissipated via electronic stopping, causing a heterogeneous re-solution, and/or through atomic collision cascades, producing a homogeneous re-solution. At the end of various decay chains, Xe isotopes are the main gaseous FPs.

In this talk, we will explore the heterogeneous re-solution of Xe bubbles in UO_2. Molecular dynamics (MD) simulations with recently-developed empirical potentials are performed to study the response of the system to ionizing FPs within the thermal spike approximation. In this approximation, a portion of the total electronic stopping power S_e is taken as the thermal spike energy through a ratio variable ζ. The probability of a Xe atom to be re-solved is then quantified as a function of bubble radius R, off-centered distance r (denoting the shortest distance between the bubble center and the cylindrical axis of the FP path), and ζ. Trends in the probability are observed, which allow for the construction of a parametric model of re-solution rate.

In the later part of the talk, evaluation of the re-solution rate model for fission of U-235 with thermal neutrons will be presented. For the evaluation, the fission product yields are taken from the JEFF-3.3 and ENDF/B-VI databases, while the kinetic energy of FPs is taken from the EXFOR library (dataset 23014005). The decay of the stopping power over distance traveled by the FPs is considered in the model. The SRIM code is employed to simulate the stopping power decrease with distance. Comparison of the re-solution rate with published empirical values and research outlook will be presented.