Radiation Effects in Metal Oxides and Carbides

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Abstract:

While traditional UO_2+Zircaloy fuel systems have provided energy to the U.S. power grid for decades, the development of advanced nuclear reactor technologies is underway to provide safe, reliable, and competitive zero-carbon emission energy sources. Some of the primary materials being considered as additives in nuclear fuel include Cr_2O_3, Al_2O, TiO_2, SiO_2, and MgO, while SiC is being investigated as coatings of TRISO fuel particles and alternative cladding to Zircaloy in LWRs. To investigate radiation effects in these metal oxides and carbides, this talk presents the results of molecular dynamics simulations using the code package, LAMMPS, to gain mechanistic insight into defect production, clustering, evolution, and annihilation in the ceramics of interest. The MD simulation results of primary knock-on atoms and projectiles up to 100 keV are also compared to *in situ* TEM ion beam irradiation experiments carried out at Sandia National Laboratories.

The key objectives of this talk are:

- Show that the most appropriate interatomic potentials to use for investigating irradiation effects in metal oxides are fixed-charge, pair potentials for their high accuracy and transferability for modeling various structural properties, equations of state, phase transitions, and defect formation energies, as well as modest computational requirements.
- Demonstrate that averaging the MD simulation results of the TDE over several crystallographic directions is appropriate due to the varying nature of collisions, including oxygen-oxygen, metal-metal, and oxygen-metal collisions, and accounting for low- and high-index directions.
- Show that increasing the PKA or projectile energy in MD simulations increases the extent of the damage cascade, and depending on the crystal structure, can:
    - Increase the number of small defect clusters rather than increasing the size of any individual cluster (e.g. SiC).
    - (b) Increase the size of a single defect production core (e.g. TiO_2)
- Demonstrate that defect production is directly correlated with the change in system potential energy in the MD simulations, both during the ballistic and annealing phases of interaction.
- Show that despite the large temporal differences between MD simulations and *in situ* TEM ion beam irradiation, the use of high enough PKA or projectile energies using MD simulations qualitatively represents observed changes from single ion strikes.
- Indicate that simulations of radiation damage with multiple ions gives more realistic results than attainable with single projectiles that could be related to potential applications.

Bio:

Ben Cowen received his B.S. in Mathematics from North Carolina State University in 2012. Since 2013, he has worked as a graduate research assistant at the Institute for Space and Nuclear Power Studies in the Nuclear Engineering Department at the University of New Mexico, under the supervision of Professor Mohamed El-Genk. His work in near-threshold and high-energy molecular dynamics simulations of numerous irradiated materials, and his parallel efforts performing *in situ* ion beam irradiation experiments at the Ion Beam Laboratory at Sandia National Laboratories, have contributed valuable material design guidance for an emerging class of ceramic nuclear fuel additives. While his graduate career at UNM is coming to a close, Ben is starting a post-doc position at Sandia National Laboratories September 17th, in which he hopes to remain in close contact with the university.