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Chemical and heat transport in uranium oxide

Marius Stan¹, Zhi-Gang Mei¹, Anders D R Andersson², John J Low¹, Alexander Thompson³, Alejandro Lopez Bezanilla¹, Christopher R Stanek², Christopher M Wolveron³ and Peter B Littlewood¹

¹Argonne National Laboratory, USA

²Los Alamos National Laboratory, USA

³Northwestern University, Evanston, USA

Modern society has increasing energy needs that require new materials with significantly improved properties. Advanced mathematical modeling and high performance computer simulation, coupled with experimental validation, contribute to enhancing the understanding of the complex phenomena that occur in materials at multiple time and length scales. This presentation reviews recent computational materials science results focused on improving the understanding of heat and chemical (oxygen, fission products) transport in uranium oxide – a ceramic material of high importance for nuclear energy applications. After a brief description of the multi-scale methodology – density functional theory (DFT+U), molecular dynamics (MD), and continuum (FEM) methods – recent results capturing temperature effects and the impact of defects on oxygen diffusivity and thermal conductivity of UO₂ are discussed, with an emphasis on the complexity of the physics and chemistry of the material. The results show a strong driving force for oxygen interstitials to form clusters, with significant impact on the properties of the UO₂ fluorite phase and neighboring compounds. The diffusion properties are a function of the cluster size, with the large clusters exhibiting high mobility through a multi-step mechanism. Experimental validation is also examined, especially the need for dedicated validation experiments. The presentation ends with a discussion of opportunities in the high-performance computing space for improved simulations of heat and chemical species transport in ceramics in general, and in UO₂ in particular.

Biography

Marius Stan is the National Technical Director of the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program. He is also a Senior Computational Energy Scientist at Argonne National Laboratory, a Senior Fellow of the Computation Institute at University of Chicago, and a Senior Fellow of the Institute for Science and Engineering at Northwestern University. His main research interests include multi-scale and multi-physics models and simulations of heat and mass transport in ceramics and metals for energy applications.

mstan@anl.gov

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