Challenges and Strategies to Experimental Validation of Multi-Scale Nuclear Fusion PMI Computational Modeling

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Abstract

The plasma-material interface in a magnetic thermonuclear fusion device is considered to be one of the key scientific gaps in the realization of nuclear fusion power. At this interface high particle and heat flux from the fusion plasma can limit the material’s lifetime and reliability and therefore hinder operation of the fusion device. The plasma-material interface PMI is a key region in the device since material can be emitted both atomistically (evaporation, sputtering, etc.) and/or macroscopically (i.e. during disruptions or edge localized modes). Deciphering the coupling at the PMI is critical to predict performance of candidate PFCs and fuel recycling. Computational tools that model PMI are critical given the multi-scale nature of this coupling and limits to existing experimental metrology. The plasma-surface interaction computational codes serve as boundary conditions to erosion/redeposition codes which link to plasma performance codes. The limiting step in this approach to a large degree depends on the sophistication and fidelity of surface response codes. Another limiting step is the large uncertainty inherent in many of the experimental measurements involved in PMI.

Validating these computational codes with controlled, well-diagnosed laboratory experiments has been critical to fine tune reliability of these codes and to aid understanding of physical mechanisms at the PMI. However, as these computational codes have limits, so do the experiments. Key is to understand the limitations of each and identify regions of validation (e.g. incident particle energies, surface mechanisms, temperature, characteristic time, etc.) and more importantly strategic problems to solve. Transitioning from heuristic models that attempt to establish phenomenological understanding of the PMI to computational tools able to predict behavior remains elusive. However, key advances in atomistic computational models and in-situ well-diagnosed simulated experiments that replicate conditions found at the fusion PMI is opening opportunities to begin unraveling the mechanisms that drive plasma-driven modification of candidate materials and their effect on plasma performance. In this work a few examples are given where the combination of atomistic computational models, in-situ facilities and PMI diagnostics demonstrate the importance of combining these tools to optimize validation at the PMI. Examples include work with lithiated graphite and irradiated tungsten. Results shed light on critical gaps in our understanding of the surface response and nano-to-microstructural deformation behavior motivating pathways for improved theoretical and computational modeling strategies as well as uncertainty quantification approaches in fusion PMI.
Biography

Prof. Jean Paul Allain completed his PhD degree from the Department of Nuclear, Plasma and Radiological Engineering at the University of Illinois, Urbana-Champaign. He received a M.S. degree in Nuclear Engineering from the same institution. Prof. Allain joined Argonne National Laboratory as a staff scientist in 2003 and joined the faculty in the School of Nuclear Engineering at Purdue University in Fall of 2007 with a courtesy appointment with the School of Materials Engineering. Prof. Allain recently joined the faculty at the University of Illinois at Urbana-Champaign in the Department of Nuclear, Plasma, and Radiological Engineering. He is an affiliate faculty with the Department of Bioengineering, the Micro and Nanotechnology Lab, and the Beckman Institute for Advanced Science and Technology. Prof. Allain is the author of over 100 papers in both experimental and computational modeling work in the area of particle-surface interactions. His research includes developing in-situ surface structure and composition evolution characterization of heterogeneous surfaces under low-energy irradiation promoting structure and function at the nanoscale. Prof. Allain was recipient of numerous awards including the DOE Early Career 2010 Award, the Research Excellence Award in 2011 and the Fulbright Award in 2015.