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Challenges and strategies to experimental validation of multi-scale nuclear fusion PMI computational modeling

J.P. Allain[a,b], C.F. Bedoya[a], A. Neff[a], M. Lively[a]

[a]University of Illinois at Urbana-Champaign, Urbana, USA

[b]Beckman Institute for Advanced Science and Technology, Urbana, USA

Email address of corresponding author: allain@illinois.edu

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 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. The plasma-surface interaction response 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. Validating these 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 heuritic models that attempt to undertstand the PMI phenomenologically 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 coatings and their effect on plasma peformance. 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 with particular emphasis on irradiated tungsten.

Tungsten and its alloys are being considered as one of the top material candidates for divertor and first-wall regions of future plasma-burning magnetic fusion reactors such as ITER. The high-density plasma in these reactors demand reliable operation under extreme environmental conditions including: multi-scale variables including: particle flux (e.g. 10^{17}-10^{24} $m^{-2}s^{-1}$), fluence (e.g. 10^{19}-10^{28} m^{-2}), temperature (200-1500 C), incident particle energies (5-1000 eV/amu) and heat fluxes (10-50 MWm^{-2}). Recent studies have observed complex surface morphology evolved when exposed to He and D/He plasmas. Extreme grain-refined tungsten has been recently suggested as a candidate plasma-facing component material with possible radiation-resistant properties. A systematic study ranging from early-stage He irradiation conditions to fusion reactor-level plasmas has been conducted. Early-stage studies include in-situ TEM analysis of He-irradiated nanostructured tungsten. Simulated conditions in future fusion plasma-burning devices are replicated using Pilot-PSI plasmas at DIFFER. 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.