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

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Motivation

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 core 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, do the experiments. Understanding the limitations of each, and identifying regions of validation (e.g. incident particle energies, surface mechanisms, temperature, characteristic time, etc...) and more importantly strategic problems to solve is vital to making progress in a credible understanding of the PMI. Transitioning from heuristic models that attempt to understand 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 unravelling the mechanisms that drive plasma-driven modification of candidate materials and coatings and their effect on plasma performance.

Key gaps in computational modeling validation

Past plasma-material interaction research has been predicated on a paradigm of approaching PFC research with emphasis on the effect of the emission of material to plasma edge performance with limited attention given to how materials properties evolve and respond to the interaction with the plasma. More importantly, novel materials synthesis that mitigate issues related to modification by high-intensity plasma has received even less attention. Furthermore, sub-surface effects indirectly impacted by long-term irradiation mechanisms and bulk effects from neutron-induced damage as would be expected in future burning plasma devices is also poorly understood and clearly an area where computational modeling and its validation is critical to establishing an integrated understanding of the PMI.

In particular for the PMI, past PFC research with off-line experiments has not emphasized investigation of the first few nanometers of a surface where the predominant particle migration and “communication” with the plasma sheath takes place. For example, a 100 eV He energetic particle penetrates roughly 10 nm into the tungsten surface. Although accelerated diffusion can occur via grain boundaries towards deeper regions in the material, ultimately the region that dictates surface erosion and recombination is at the top 10-100 nm on the surface. Surface response models (i.e. MD, TRIM, TRIDYN) are limited by their strong dependence on first hand knowledge of a potential (in e.g. MD) or bond and surface binding energies (e.g. TRIM, TRIDYN). No code exists today that can predict the ion-induced compositional evolution during irradiation which can drive the morphological evolution of the material surface. One critical challenge to validation of PMI computational codes is the strong spatio-temporal coupling that exists when plasma interacts with a material’s surface. The figure below illustrates the spatio-temporal aspects of PSI scales and the critical gaps between multi-scale modeling and experimental validation. For example, in order to capture diffusional mechanisms triggered by ion-induced effects one would require an experimental capability that is pulsed and capable to capture both by spectroscopy and microscopy.
mechanisms that cross from 100’s of picoseconds to 100’s of microseconds. Although progress has been made in areas outside of fusion with ultrafast systems, little progress has been made to design these systems with complex materials that evolve in an extreme environment such as the fusion plasma edge that includes hydrogen isotopes and energetic particle implantation. This challenge also limits the ability to validate models in these time scales. Another challenge is the vast energy scales involving the PSI. For example, hyper-thermal atoms (e.g., deuterium in the private flux region) can induce molecular changes on the first few monolayers of a material that also can be irradiated by higher energy particles that together can drive compositional changes in plasma-facing surfaces. Furthermore, erosion/re-deposition processes result in deposited thin-films with a composition that can be dramatically influenced by the various energetic particles that interact with these surfaces.

**Recommendations**

The dynamic PSI environment requires novel characterization that goes beyond conventional approaches to surface science. Conventional approaches seek to simplify conditions of material surfaces in order to establish controlled, model systems to couple to existing computational models. This however is only the first step and arguably can only go so far to describe the real environment materials are subjected in the PSI. Here we characterize “in-situ” to be a measurement conducted “in place” of where the test sample is characterized in the time-scale of modification by the incident irradiation. This time scale is dictated primarily by the prompt or ballistic time-scales moving to thermal or diffusional effects and finally PSI time scales. In practice the plasma-material interface is constantly reconstituted resulting in complex mixed material systems.

We recommend a strategic approach at computational validation by identifying complementary in-situ techniques that can be coupled to multi-scale computational modeling. One example includes in-situ irradiation modification coupled to high-resolution microscopy and spectroscopy that can couple both the compositional and morphological evolution of mixed materials relevant to the fusion PSI. Complementary techniques can use pulsed probes coupled to irradiation-driven triggers that can provide compositional and morphological information needed for validation. The materials in question should be relevant in the most general sense for example examining tungsten and tungsten-based alloys to more chemically active systems that include lithium. Irradiated materials and coatings can also be included in such an effort that can partially provide a surrogate environment with large-scale fluence damage exposed, for example, in plasma linear devices with appropriate plasma flux and fluence parameters.