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Review article

Unraveling the surface chemistry processes in lithiated and boronized plasma material interfaces under extreme conditions

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Abstract

The review of recent theoretical and experimental research on the complex surface chemistry processes that evolve from low-*Z* material conditioning on plasma-facing materials under extreme fusion plasma conditions is presented. A combination of multi-scale computational physics and chemistry modeling with real-time diagnosis of the plasma-material interface in tokamak fusion plasma edge is complemented by ex-vessel *in-situ* single-effect experimental facilities to unravel the evolving characteristics of low-*Z* components under irradiation. Effects of the lithium and boron coatings at carbon surfaces to the retention of deuterium and chemical sputtering of the plasma-facing surfaces are discussed in detail. The critical role of oxygen in the surface chemistry during hydrogen-fuel irradiation is found to drive the kinetics and dynamics of these surfaces as they interact with fusion edge plasma that ultimately could have profound effects on fusion plasma confinement behavior. Computational studies also extend in spatio-temporal scales not accessible by empirical means and therefore open the opportunity for a strategic approach at irradiation surface science studies that combined these powerful computational tools with in-vessel and ex-vessel *in-situ* diagnostics.

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1. Challenges of plasma-material interactions exposed to fusion plasmas

The interactions of a thermonuclear tokamak plasma and the bounding material surface are inherently extreme. Providing energy from nuclear fusion and in particular, confining magnetically hydrogen isotopes to sustain the reaction is one of the grand challenges of today. Energetic charged, excited, neutral and neutron particles interact with a material surface that is constantly evolving under extreme conditions of heat, pressure, radiation and stress. This dynamic interaction results in the combination of two disciplines: plasma physics and material-surface science, resulting in one of the most challenging areas of multidisciplinary science. Plasma-material interactions (PMI) have an important role in the operation of a fusion reactor due to the high particle flux and heat-flux from the fusion plasma resulting in damage of the plasma facing components (PFCs), limiting their lifetime while the sputtered material effecting cooling the core plasma. One consequence of complex plasma-material interactions is the effect on the plasma edge pedestal where steep gradients of density and temperature of the electrons in the plasma can be significantly affected by the impurity flux and the recycling of hydrogen fuel from the wall surface. The PMI has multiple spatio-temporal fundamental processes and synergies [1—5]

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driven by both the plasma on one side of the interface and the material transformation on the other. A major goal in PMI science is to extend high-performance plasmas for very long durations and to integrate this performance with PFCs that can withstand high heat and particle fluxes while maintaining structural integrity and controlling retention of fusion fuel [6,7]. The nuclear fusion plasma-material interaction provides an environment where both the radiation and matter interaction are at extreme conditions. Extreme conditions are here defined as those that drive matter far from equilibrium and in some cases "very far" from equilibrium. For example, current fusion tokamak experimental devices with power extraction levels between a few MW/m^2 are for the former case and those above 25−50 MW/m^2 heat fluxes with radiation damage of several tens to hundreds of dpa (displacements per atom) for burning-plasma fusion reactors, are for the latter case. Among the most elusive technical challenges for the advancement of thermonuclear magnetic fusion energy is the predictive control of hydrogen recycling in the PFC materials as well as the management of erosion and defects induced by plasma particle and neutron irradiation and these effects on plasma confinement [8,9]. One of the critical knowledge gaps is an understanding of the changes in surface composition and chemistry at the atomic-to-nano spatio-temporal scales in the extreme conditions in tokamak fusion plasmas. The non-linear coupling of energetic particles and the material surfaces that continually evolve under the extreme conditions of a tokamak plasma makes it difficult to measure and let alone predict material behavior. By establishing an understanding of the plasma-material interaction one would ultimately begin to establish links to overall tokamak machine performance across both time and spatial scales combining real-time measurements in these extreme environments. The tools of which would include validating advanced computational PMI codes with well-diagnosed *in-situ* facilities and connecting these results to provide tendencies and qualitative behavior that can guide materials design and tokamak operation regimes. Although there has been historically a recognition of the importance of plasma-material interaction in fusion tokamaks, the majority of the work has been inherently Edisonian with very limited capability to capture the dynamic, evolving material surface.

Both low and high Z choices for plasma facing surfaces (PFS) in present tokamak fusion devices have significant performance issues [4,5,10,11]. PMI research in the National Spherical Torus Experiment (NSTX) and its Upgrade (NSTX-U) of the Princeton Plasma Physics Laboratory is focused on testing a variety of PFC candidate materials including low-Z coated graphite, high-Z materials (W, Mo) and liquid metals. Although carbon has been down selected as a viable future plasma-burning fusion reactor wall material [12], it remains the primary material component in most existing experimental tokamak devices. Therefore, devices that study unique plasma confinement regimes and boundary plasma effects such as the work in NSTX-U leverage the use of wall conditioning techniques as enabling technologies. The conditioning of plasma facing carbon components by lithium and boron is an important part of this research effort and it has led to the improved performance in fusion reactor experiments [13,14]. This has included numerous pioneering research efforts on complex PMI surface chemistry and physics validated in NSTX plasma regimes [6,7,15−20].

The combination of high-energy, high heat-flux and the complex evolution of material surfaces exposed to tokamak plasmas result in deciphering mechanisms under extreme conditions with sophisticated experimental and computational tools. The work of Allain and Krstic is to couple experimentally-validated multiscale theory and simulation, starting from mutually verifying quantum mechanical and classical atomistic computations to study the dynamics of the creation and evolution of the plasma material interface under irradiation by atoms and molecules at boronized carbon, lithiated carbon, boronized-lithiated carbon, with both solid and self-healing liquid metals (e.g. lithium). The time scale of most of the surface chemical and topology changes is in the picosecond to nanosecond range of the atomistic approaches. The goal of this review is to provide a bottom-up understanding of phenomenology and predictive tools necessary for successful design of the relevant laboratory experiments of plasma-particles retention, sputtering, reflection and morphological changes in extreme conditions, as well as the input parameters for the source and sink terms in appropriate nano-to-mesoscale modeling.

Conditioning of PFCs is an important enabling procedure for tokamak operation [14]. A major challenge for magnetic fusion devices generally is to extend high-performance plasmas for very long duration, and to integrate this high performance with PFCs that can withstand very high heat and particle fluxes while maintaining structural integrity with controllable retention of fusion fuel in a severe fusion reactor environment. Conditioning with boron and lithium has led to improved performance of a variety of experimental fusion machines [15,21]. In NSTX-U wall conditioning with boron was used to provide fuel density control and impurity reduction [15,16]. NSTX-U is comprised of mostly carbon-based PFCs (i.e., ATJ graphite tiles) as stated earlier. Traditionally boron has been applied to the first wall of magnetic confinement machines via plasma-enhanced chemical vapor deposition (PE-CVD), using mixture of a buffer gas (e.g. He) and a gas that contains B atoms (e.g. diborane (B_2H_6) or trimethylborane ($B[CH_3]_3$)) [22].

Recent work with lithium coatings evaporated on a variety of metallic and graphitic surfaces in over ten tokamak fusion machines around the world, has provided an evidence of the sensitive dependence of plasma behavior on lithiated plasma facing surfaces [23−25]. Thus, in NSTX, Li evaporation decreased the H-mode access power threshold, increased the stored energy and allowed longer plasma discharges when compared with plasma discharges without Li conditioning [21]. These improvements have been correlated to the reduction of impurities and with the reduction of fuel recycling with the formation of Li-O-D complexes [17]. In addition, He-glow discharge (He-GDC) approaches have also been used together with wall conditioning using B or Li depending on the desired performance conditions of NSTX plasmas [26]. In this work

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