Fundamental science of the synergy of multi-species interactions in a high plasma-heat-flux environment

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Introduction. In the recent Greenwald Report [1], areas of urgent knowledge gaps toward developing a magnetic fusion demonstration reactor were identified. These include plasma-facing components (PFC's), plasma-wall interactions (PWI's), and fusion materials.

All three areas were identified as requiring major extrapolations from the present knowledge base, with no solutions in hand or with solutions foreseen but not yet achieved. Plasma-surface interaction (PSI) science is strongly linked to all these areas. The choice and deployment of plasma-facing materials should be optimized to ensure the performance and sustainment of the burning plasma, and therefore depends on PSI science knowledge to design and build viable heat-bearing components. An important issue for the fuel cycle is the retention of tritium fuel in the PFC materials; this is a current subject of study in plasma-surface interactions, but one for which orders of magnitude reduction in retention are required from present experiments to a DEMO. The third area emphasizes the strong interaction and coupling between the plasma and wall materials, and highlights the present lack of predictive capabilities.

PSI, in particular, chemical and physical sputtering, cause erosion of the limiter/divertor plates and vacuum-vessel walls, whether these are made of C, Be, W, or some combination (i.e., mixed materials). Such impurities can degrade fusion performance by diluting the fusion fuel and cooling of the core excessively via line radiation from partially ionized impurity atoms. Hydrocarbon re-deposition onto plasma-facing components can lead to long-term accumulation of large in-vessel tritium inventories via co-deposition.

The choices of wall material has profound effects on confinement of fusion-grade plasmas, assuming adequate power and particle handling of the plasma facing components and other internal components. The present knowledge of plasma interactions with these surfaces is still mainly empirical, and "wall conditioning" remains an art. Although carbon-based materials have superior thermal–mechanical properties, they are expected to trap high levels of tritium by co-deposition with eroded carbon and thereby severely constrain safe plasma operations. Thus, a mix of several different plasma-facing materials is now proposed in ITER to optimize the requirements of areas with different power and particle flux characteristics. The slow rate of progress in the area of tritium removal, together with progress of divertor tokamaks with high-Z (e.g. tungsten) walls, suggests investigations of all-metal surfaces, which are held, in case of DEMO, at elevated temperatures. The stability of the modified surfaces under high transient heat fluxes during Edge Localized Modes (ELMs) and disruptions is another important question and expands the range of plasma parameters that needs to be studied both experimentally and theoretically.

This white paper addresses the research to understand and predict individual phenomena both under well-controlled conditions as well as under more realistic large-area, high plasma heat flux conditions where synergistic multi-species interactions play significant and possibly dominant roles.

Scientific issues of synergistic interactions. The likely use of high-Z refractory metals for plasma facing materials in the DEMO reactor at sustained elevated temperatures and in continuous operation, as well as the need for efficient power conversion, raises important issues related to the tritium retention, permeation, recombination, surface erosion, chemical reactions, damage annealing, codeposition, nanostructures formation, blistering (in e.g. tungsten), and their dependences on plasma and wall temperatures, as well as plasma and neutron fluences . High wall temperatures (>600C) and high fluence conditions, in particular, have not been adequately studied to date.

The key issues for surface studies on ITER-relevant carbon based materials are erosion, reflection, impurity transport in the interacting plasma, redeposition, T uptake and removal. Specific needs [2], among others, include determination and characterization of the composition of eroded species such as hydrocarbon molecules and radicals, their rotational/vibrational state and energy spectra, and their sticking coefficients to surfaces as a function of energy.

An expansion of the available erosion database towards low impact energies (~10 eV) is needed to close the gap in erosion data between energetic hydrogenic ions and thermal hydrogenic atoms and ions, for high-Z, carbon, and mixed materials systems. Properly validated by experiments, computational simulations of the PSI would establish the needed understanding for boundary plasma modeling, filling in data and processes often not readily accessible by measurements. The multi-scale nature of the PSI requires simulations which will combine molecular dynamics (MD, including development of appropriate mixed-material potentials) at the ns time scale and the kinetic Monte Carlo (MC) processes at longer time scales. The synergistic interactions of various plasma particles (ions, atoms, molecules), having a range of impact energies and angles, with possibly hydrogenated target surfaces typical for plasma-facing divertor tiles and redeposited layers in magnetic-fusion reactors is an open and challenging field of research. For example, a small He concentration in an irradiating plasma was found to result in nanostructure modification of the plasma interface region of tungsten, suppressing blistering and deuterium retention [3]. The presence of intense neutron bombardment and resulting accumulated material damage may further significantly alter the microstructure properties of the material surface, and hence also the relevant PSI processes. The role of neutron damage in DEMO relevant PSI's involving tungsten is just beginning to attract interest.

Close collaboration of plasma-surface experiments with beam-surface experiments and modeling and computational studies is needed to interpret data and improve fundamental understanding in all such synergistic interactions. Previous findings [4] of the sensitive dependence of PSI processes on the microstructure of the target surface (for example, the hydrogenization density distribution and hybridization structure of carbon, its thermal conductivity, etc.), as well as on the type and state of the incident particles points to the need to account for the plasma composition, its irradiation fluence and irradiation history in studies of DEMO relevant materials [5].

Challenges exist not only for studying various forms of refractory metals, carbon (including crystalline and amorphous C structures, CFC's, C doped by boron, beryllium, and various heavier metals, C coated metals), new material compounds, alloys and combinations, but also for characterizing and understanding the resulting hydrogenated, damaged/modified mixed materials surfaces and particle interactions.

R&D requirements and activities. Coordinated research is required to investigate 1) the properties of the fundamental interaction phenomena involved, as well as 2) the nature of the synergistic interactions involving multiple plasma and impurity species having combinations of impact energies and angles, and the anticipated hydrogenated, plasma and neutron heated, damaged and otherwise modified wall surfaces and redeposited layers.

The first category of research will require bombardment of material surfaces and surface conditions of interest to the PSI by ionic and neutral atoms and/or molecules (H, H_2, H_3, Be, C, W, Li, He, N, N_2, O, etc.) in various isotopic forms and with controlled incident energy, species, and impact angle, typical of ion-beam experiments. Experiments and simulations carried out under such well-controlled conditions have already uncovered new details of the sputtering interaction, such as a strong dependence of the chemical sputtering yield on the vibrational excitation of the incident molecule [6] as well as on the atomic vs. molecular nature of the impinging ion [7]. This research at the fundamental level, applied to both tungsten and carbon surfaces, will aim to establish the scientific basis needed to guide the second research category.

The second category of research will require at minimum a high plasma heat and particle flux environment with recycling plasma conditions typical of the tokomak divertor region. The plasma size scale should be larger than the recycling plasma and impurity mean-free-paths. The plasma duration needs to be longer than the time scales of the longest anticipated physical mechanisms of interest. Time constants related for example, to the formation and sustainment of redeposited microstructure layer and its dependencies on several other simultaneous processes will have to be measured and determined for the first time. A high priority requirement of experimental set-ups will be unprecedented access for measurements of the many elements of the synergistically interacting phenomena, and for convenient replacement of the plasma facing component modules.

It is further desirable to have the capability to apply ms duration heat pulses that are at least an order of magnitude larger than the continuous heat fluxes. This would enable research into such phenomena as material ablation, melt layer formation and dispersal, impurity radiation shielding, and their roles in determining the lifetimes of interest.

Below are listed example elements of the research thrust:

Fundamental Processes: Controlled particle beam experiments (H^+, H_2^+, H_3^+, D^+, D_2^+, He^+, D_3^+) and corresponding MD/MC computer simulations of refractory metal (e.g. W) or selected graphite surfaces at various temperatures, for impact-energy/impact-angle/impact-particle dependence of erosion, blistering (in the case of metals), hydrogen retention, reflection and re-emission, hydrocarbon sputtering and total C erosion (in the case of carbon containing or coated materials) in the not-well characterized region of low impact energies (1-100 eV); Possible experimental probes of the surface processes include time-of-flight and/or quadrupole mass spectrometry, visible and IR spectroscopy, laser induced fluourescence, quartz crystal microbalance, ellipsometry, and thermal desorption spectrometry. Ex-situ diagnostics include weight-loss measurement, UV and visible Raman spectroscopy, scanning electron and Auger microscopy, X-ray induced photospectroscopy, and atomic force microscopy. The development and improvement of the interaction potentials for mixtures of the above-mentioned materials (H, He, W, C, Be) is imperative for improved predictive capabilities and will be of high priority in the theoretical/computer simulation research.

Synergistic interactions. Studying the same processes (sputtering, erosion, hydrogen retention and permeation, blistering, etc) using plasma irradiation, again for selected refractory metal or graphitic surfaces at various temperatures, gives rise to synergistic effects from the broadened energy and angular distributions, and the multi-specie nature (ions and neutrals, atoms and molecules, H and He, etc.) of the impinging plasma. While similar probes of the PSI processes could be used as with the beam irradiation case, significant additional effort would be needed to characterize the irradiating plasma (using reciprocating Langmuir probes and retarding field analyzers, visible and infrared spectroscopy, etc.), as well as to accurately characterize the temperature profile of the target area exposed to large heat fluxes (e.g., using two-color pyrometry in conjunction with thermocouple measurements).

With the same requirements for the beam, plasma and sample characterization and diagnostics, experiments can be done with ex-situ prepared or “plasma sprayed” samples that would help assess the material synergy effects, such as of W deposits on carbon as well as mixed material design. This could include carbon or W samples with deposited W or C, implanted W/Be, as well as pure metal (W, Be) samples, as well as studies of the PSI processes associated with neutron damaged material samples.

References:

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