Synergistic Effects of Radiation Damage and Plasma-Material Interactions

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1 Synopsis

ITER will have very low neutron fluence and displacement-per-atom (dpa) levels compared to DEMO. Thus, for ITER, issues pertaining to radiation damage and plasma-material interactions (PMI) are generally decoupled. However, for DEMO, this will no longer be the case. The large neutron fluence and associated radiation damage expected in DEMO will alter the bulk properties of plasma facing components (PFC's), which in turn can impact PMI phenomena that depend on PFC temperature and tritium retention/permeation. The synergistic effects of radiation damage and PMI likely to arise in DEMO cannot be truly studied in an integrated manner until a high duty cycle burning plasma device like FDF/CTF is built and becomes operational. In the present domestic fusion development path, this is about two decades away. However, we have other existing (*e.g.*, ion beam irradiation and plasma exposure) and nearer-term proposed facilities (*e.g.*, IFMIF or MaRIE/FFMF[1]) that could be used in conjunction with each other, as well as coordinated multi-scale modeling, to address this issue sooner while informing the engineering design for FDF/CTF.

This white paper is organized as follows. Section 2 briefly summarizes the likely synergistic effects of radiation damage and PMI. Section 3 describes the scientific and technical requirements for addressing this issue. Section 4 proposes several research thrusts.

2 Synergistic effects of radiation damage and PMI

Neutron irradiation of a material causes atomic displacement damage, vacancies and interstitials, defect clusters, helium production and accumulation, and alloying due to transmutation. This can lead to material swelling and embrittlement, as well as changes in bulk material properties such as thermal conductivity and tritium trapping and permeability. For low-activation structural materials, the key issues are maintaining dimensional stability and mechanical integrity. For PFC's, however, the key issues are understanding how the consequences of neutron damage affect temperature-dependent chemical processes such as surface erosion/redeposition and tritium retention/permeation, as well as the ability of the PFC to withstand thermal shock associated with disruptions or large edge localized modes (ELM's).

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[1]MaRIE: Matter Radiation Interactions in Extremes, LANL's proposed signature science facility; FFMF: Fission Fusion Materials Facility, a spallation neutron source that is part of MaRIE.

The synergistic effects of radiation damage and PMI are recognized in the Greenwald Report. For plasma-wall interactions, the report states "it will be necessary to have a predictive model capable of accurately forecasting both the edge plasma conditions and the response of the plasma facing material to the fusion plasma" (p. 170). For tritium retention, the report states: "Neutron radiation damage occurs throughout the thickness of materials and creates sites where T can be retained. The synergistic effects of high plasma particle flux and neutron damage have never been studied" (p. 172). Finally, for characterization of tritium permeation, the report states: "Permeation barriers seem to work well in the absence of neutron irradiation, but development is needed for nuclear applications" (p. 174).

3 Scientific and technical requirements

To develop a predictive capability for assessing the synergistic effects of radiation damage and PMI on PFC's, and to come up with novel materials solutions, will require a concerted multi-scale modeling effort, abundant experimental validation, and a materials synthesis capability guided by first-principles understanding of the causes of relevant material property degradation.

Multi-scale modeling: The ultimate goal is the integrated dynamical modeling of the plasma-boundary system from the scrape-off layer (SOL) to the sheath to the PFC surface and finally to the material bulk behind the surface. Each system requires a different modeling tool with different time/length scale requirements and physics packages. They each need to be validated with experimental data and eventually coupled together.

Material exposure to DEMO-relevant radiation and PMI environments and in situ characterization: Prior to the availability of FDF/CTF, there are several potential ways to address the synergistic effects of radiation damage and PMI, listed here in order of availability:

1. (a) Serial exposure of PFC materials to multiple ion beam irradiation (to achieve DEMO-relevant dpa-damage and dpa-to-helium ratios with in situ ion beam analysis of the material) and to high heat flux plasmas (for PMI); the serial exposure approach could be undertaken, for example, at the LANL Ion Beam Materials Facility (IBML) and then at the UCSD PISCES facility. These facilities already exist and are operational. (b) Simultaneous exposure to multiple ion beam irradiation and high heat flux plasmas by adding a PMI facility to an existing multiple ion beam facility.

2. Serial exposure of PFC materials, *i.e.*, first to neutron irradiation (at an accelerator-based irradiation facility) to a specified dpa level and with reactor relevant helium-to-dpa ratios, and then to PMI at a separate facility (with hot cell capability). This approach requires the availability of IFMIF or MaRIE/FFMF; the latter can be available in as soon as 5 years.

3. Simultaneous radiation damage and PMI exposure by co-locating a PMI facility with an accelerator-based neutron irradiation facility. This option may be technically difficult to implement; much work would be needed to assess this possibility. If feasible, then this capability could also become available on the 5 year time frame.

For all these options, in situ characterization is needed to develop first-principles understanding of damage/PMI phenomena and their dynamics, and to provide the best validation data.

Material innovation, synthesis, testing, and characterization: It would be desirable to harness modern materials synthesis capabilities to develop tailor-made materials designed to excel at particular functions, and to test and characterize these materials in the above exposure environments. As an example, recent studies[2] at LANL showed that copper-niobium multi-layer composites with

[2]M. J. Demkowicz et al., Nucl. Instrum. Methods Phys. Res. **B261**, 524 (2007).

layer thicknesses as small as 4 nm demonstrated remarkable resistance to radiation damage at room temperature, and it was found that the fraction of retained helium decreased significantly when layer thickness was increased to 40 nm. This implies that the interfaces between Cu and Nb serve as efficient helium sinks since the 40 nm structure contains more interfaces than the 4 nm structure. The studies also showed that when the Cu-Nb composite material was implanted with helium ions at high temperatures, the fraction of retained helium was found to decrease. The fact that no ruptured blisters were observed by scanning electron microscopy on the surfaces of these samples suggests that the interfaces between Cu and Nb layers might have served as pathways for fast helium diffusion out of the material. Such features could potentially also provide an efficient way to release trapped tritium in PFC's.

4 Proposed research thrusts

Theory/modeling: While the SOL and PFC surface erosion/redeposition have received considerable attention, understanding the role of the sheath in regulating PMI and larger-scale atomistic simulations of the bulk material are both ripe for advances. For the sheath problem, theoretical models of quiescent and dynamic sheaths, taking plasma turbulence into account, must be developed, and detailed turbulent ion/electron transport can be quantified via large-scale particle-in-cell (PIC) simulations (*e.g.*, using LANL's fully electromagnetic VPIC[3] code on the supercomputer Roadrunner). For modeling the response of the bulk material to radiation damage, molecular dynamics modeling (MD) provides detailed information on the energetics of point defect migration to/within interfaces and grain boundaries and also the stability of layered structures. Accelerated MD techniques[4] are now available to model how vacancies annihilate, migrate, and form various defect types on time scales longer than nanoseconds.

Material exposure, testing, and characterization: A research program focusing on material exposure studies according to option #1(a) listed above can be initiated immediately, with #1(b) available within a few years if the need for it is scientifically justified. Modeling should be used to determine the most faithful way of simulating DT neutron damage using (multiple) ion beams for achieving relevant dpa-to-helium ratios. For option #2, some key issues need further study to determine the relevance of serial material exposure to the integrated radiation damage and PMI environment of CTF/FDF/DEMO. These issues include the need to understand the "quasi-equilibrium" states reached by materials at different dpa and helium-to-dpa ratios, the time scales for reaching and departing from these states, and the coupling of these time scales to PMI time scales. Assessment of these issues will allow us to determine the extent to which serial exposure is a relevant approach, and how much time can be allowed to elapse before moving a sample from the damage to the PMI environment. It is likely that certain damage/PMI phenomena can be studied meaningfully with a serial approach, but that other phenomena will require option #3 as the only viable testing approach ahead of FDF/CTF. For all these studies, we emphasize in situ characterization of both materials damage processes and PMI phenomena.

Novel materials synthesis and testing: Finally, we advocate a shift in paradigm from materials "observation and validation" to "prediction and control." Based on findings coming from the above two research thrusts, new materials such as specialized composites or with engineered nanostructures should be designed and fabricated and then tested/characterized in the available exposure environments. Their performance will then be fed back to the models, and the design can be improved iteratively. We can leverage DOE/BES funded capabilities, such as LANL's Center for Integrated Nanotechnologies (CINT) user facility, for the design and fabrication of novel specialized materials.

[3] K. J. Bowers et al., Phys. Plasmas **15**, 055703 (2008).
[4] A. F. Voter et al., Annu. Rev. Mater. Res. **32**, 321 (2002).