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Advanced simulation of mixed-material erosion/evolution and application to low and high-Z containing plasma facing components

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ABSTRACT

Plasma interactions with mixed-material surfaces are being analyzed using advanced modeling of time-dependent surface evolution/erosion. Simulations use the REDEP/WBC erosion/redeposition code package coupled to the HEIGHTS package ITMC-DYN mixed-material formation/response code, with plasma parameter input from codes and data. We report here on analysis for a DIII-D Mo/C containing tokamak divertor. A DIII-D/DiMES probe experiment simulation predicts that sputtered molybdenum from a 1 cm diameter central spot quickly saturates (~4 s) in the 5 cm diameter surrounding carbon probe surface, with subsequent re-sputtering and transport to off-probe divertor regions, and with high (~50%) redeposition on the Mo spot. Predicted Mo content in the carbon agrees well with post-exposure probe data. We discuss implications and mixed-material analysis issues for Be/W mixing at the ITER outer divertor, and Li, C, Mo mixing at an NSTX divertor.

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1. Introduction

As discussed in e.g., [1,2] mixed-material plasma facing component (PFC) surfaces can obviously arise from sputtering, transport, and deposition of two or more materials. It is important to model this accurately to explain and predict PFC performance. Rigorous, predictive analysis ultimately requires full-surface, self-consistent, micro-resolved, coupled calculations for time-dependent plasma particle impingement, sputtering, impurity transport/redeposition, and surface evolution. We are progressing to such goal using the REDEP/WBC full-kinetic, 3-D, impurity sputter/transport code package [3] coupled to the ITMC-DYN composite/mixed-material response and 3-D surface evolution code [4], and using near-surface plasma inputs from codes and data.

The DIII-D/DiMES experiment of August 1, 2011 [5,6] was designed to study high-Z material erosion/redeposition and hopefully validate predictions of high redeposition. Because the experiment involved a very small Mo spot in a large C divertor it has proven critically important to understand the resulting Mo/C mixing, re-sputtering, and transport. Our analysis explains the key observed results of high spot Mo redeposition, Mo content in the carbon portion of the probe surface, and Mo transport to off-probe areas.

We do observe a code/data discrepancy in upstream/downstream redeposition profiles, and it is likely that future petascale type analysis would be needed to resolve this. Such analysis will also be required for other mixed-material devices, such as ITER and NSTX, with large area components and multiple low and high-Z plasma facing materials.

2. Molybdenum/carbon DIII-D DiMES probe modeling

2.1. Problem description

The DiMES experiment used a 1 cm diameter 24 nm thick central Mo spot, on a 5 cm diameter graphite probe, exposed to 28 total seconds (7 shots × 4 s/shot) of steady-state phase plasma impingement at the DIII-D divertor outer strike point. Post-exposure analysis of the probe by RBS determined a net Mo spot erosion rate of 0.42 nm/s and Mo content in the probe carbon of 19% of the eroded material [6]. Although Mo–I photon emission spectroscopy was performed to measure the in situ gross erosion rate, this was found subject to large uncertainties [5]. Thus, we rely on the post-exposure probe analysis, for our main code/data comparisons.

2.2. Simulation method

REDEP/WBC code package analysis is described generally in e.g., [3] and for a past DIII/DiMES experiment in [7]. Briefly, WBC computes the 3-D, 3-V, sub-gyro-orbit, full-kinetic motion of sputtered atoms/ions in the edge/SOL plasma, subject to Lorentz force motion, and velocity-changing and charge-changing collisions with the plasma.

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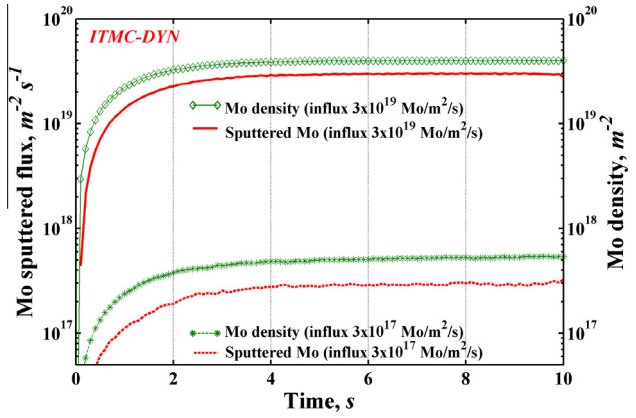

Fig. 1. Time-dependent sputtered Mo flux and areal density from/in DIII–DiMES carbon probe surface, for 3×10^{19} m^{-2} s^{-1} and 3×10^{17} m^{-2} s^{-1} incident Mo ion flux. WBC/ITMC simulation.

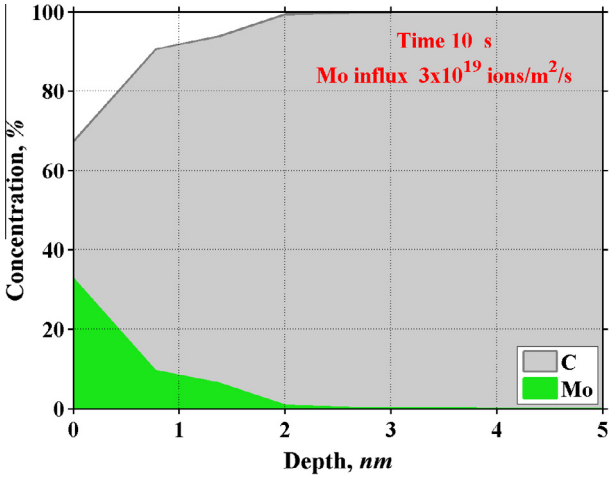

Fig. 2. Mo and C surface composition in DIII-D/DiMES carbon probe surface, at 10 s, for 3×10^{19} m^{-2} s^{-1} incident Mo ion flux. WBC/ITMC simulation.

We compute pure Mo sputtering and Mo/C dynamic surface composition/response using the HEIGHTS package ITMC-DYN code. ITMC-DYN is a binary collision approximation (BCA) code which considers elastic and inelastic interactions of ions and atoms in materials, as described in [4]. The code accounts for changes in target composition due to time-dependent processes of ion penetration and mixing, scattering, reflection, physical and chemical sputtering of composite materials, dynamic surface evolution, thermal diffusion, hydrogen isotope molecular recombination, and surface segregation. Variable input to ITMC-DYN, for this study, is the incident Mo ion flux; with D and C fluxes being constant in space and time.

Full-resolution, ultimate coupling of the codes – for future full-rigor predictive purposes – would involve running ITMC-DYN for every spatial computational point, at every time step, with micro convolution over the REDEP/WBC-supplied local incident ion velocity distribution – giving among other things, time and space-resolved sputtered atom velocity distributions. This would require advanced, real-time, petascale supercomputing; beyond the scope of the present effort. Instead, we employ a reduced method using average incident ion velocity values and related numerical techniques. For example, we use two (and not several hundred) sputtered Mo atom velocity distributions from ITMC in WBC, viz., for (1) pure Mo sputtering, and (2) for Mo/C mixed material sputtering (such distributions being substantially different, e.g., with the latter distribution having higher average sputtered energy due to lower surface binding energy and different collision cascade kinematics). This reduced approach is adequate for the present goal of explaining broad observed trends, and also because of the small areas involved, with correspondingly small plasma parameter variation. Full-resolution simulations will be needed for future work, including for fusion devices with highly spatially varying plasma parameters, and/or to resolve remaining code/data discrepancies in DIMES probe experiments, such as toroidal deposition profiles, both points to be discussed.

Plasma conditions for the DIII-D simulation are based on inputs from the Langmuir probe-calibrated OEDGE code per work of Elder, Stangeby et al. [5]. The background plasma is a D plasma with carbon impurity, with reference time-averaged temperature/density flat-top values at the sheath/plasma boundary of $T_e = T_i = 30$ eV, $N_e = 1.5 \times 10^{19}$ m^{-3} (essentially uniform over the probe surface to within experimental error and fluctuations), with D and C particle impingement determined from sound speed flow and magnetic field geometry data. Carbon content in the plasma was not precisely measured but is estimated at 1% of the D content [5], with characteristic C^{3+} state at the near-surface outer divertor region. (Results are found to be not fundamentally different for a range of carbon charge states). The BHI-3D sheath code [8] was used to verify WBC models for the DIII-D divertor dual-structure, magnetic and Debye sheath, including incident ion average impingement energy/angles for the experimental conditions – these being approximately 150 eV (D^+), 400 eV (C^{3+}), both at 50° elevation angle incidence (from normal), and peaked in the downstream (along toroidal magnetic field/plasma flow) direction in aziumthal angle.

In the coupled simulation Mo atoms are launched randomly from the 1 cm diameter spot per ITMC-DYN energy and angle probability distributions for C on Mo sputtering (D energies being mostly below the pure-Mo sputter threshold). Mo ionization and transport is then followed. An ion history terminates if redeposited on the Mo spot (self-sputtering being a small effect here), or deposited off-probe. A Mo ion incident on the probe carbon is re-sputtered per ITMC-DYN calculation, which also takes into account the simultaneous D ion flux. A run uses 10^6 histories, with spot-sputtered particle numerical weighting calibrated to the measured net erosion rate of 0.42 nm/s. Key simulation outputs are redeposition rates, gross/net erosion ratio, and Mo content in the carbon.

2.3. Results

All parts of the DiMES probe surface are predicted to undergo net erosion. About half of the spot-sputtered Mo is transported to the initially-carbon surface, with resulting mixed-material Mo/C formation, C sputtering, and Mo re-sputtering. Erosion rates for this probe region outside the central Mo spot vary spatially from about 3–6 nm/s, or about 10× higher than the pure Mo spot itself. The mixed-material erosion rate depends on the incident Mo flux, with maximum erosion occurring where incident Mo flux is the least, i.e. where the surface remains mostly carbon.

Figs. 1 and 2 show the time-dependent sputtering flux and areal density of Mo from/in the evolving mixed Mo/C surface, for two typical (high and low) values of incident Mo flux; these occurring near and farther from the spot, respectively. Initially the surface is pure C and then becomes enriched in Mo, with related increase in Mo sputtering. Mo builds up in the (receding) surface to a depth of about 1–2 nm. A steady-state surface composition is reached at about 4 s – about independently of Mo flux – and short compared to the 28 s total exposure time.

Fig. 3 shows sample computed trajectories of sputtered Mo. The trajectories show an approximately straight line motion from sputtering to first ionization, and then generally both simple and complex patterns of ion gyro-rotation, charge-changing and

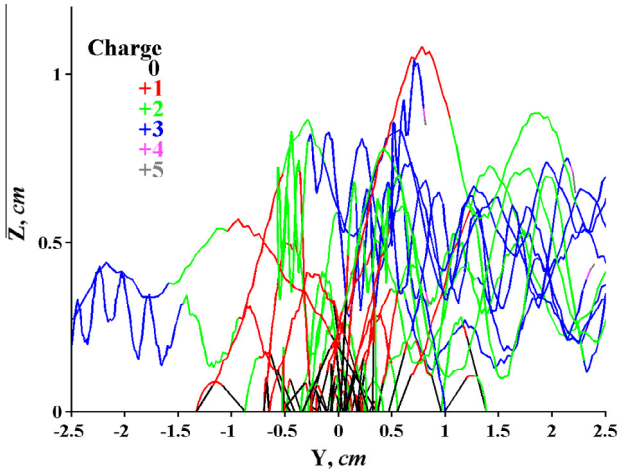

Fig. 3. Typical sputtered Mo trajectories (50 histories), 2-D plot. Y = toroidal direction through probe center, Z = distance above probe. (Trajectory segments continuing past 2.5 cm radius probe dimension not shown.).

Table 1
REDEP/ITMC analysis summary for DiMES probe sputtered Mo (10^6 histories).

Parameter	Value
Ionization mean-free-path[a]	1.2 mm
Charge state[b]	1.7 (0.73)
Energy[b]	156 (86) eV
Incidence elevation angle (from normal)[b]	22 (11)°
Transit time[c]	.98 μs
Redeposition fraction on Mo spot	.54
Redeposition fraction on divertor[d]	1
Mo content in carbon portion of probe; at end of discharge	$.79 \times 10^{16}$ atoms

[a] For sputtered Mo atoms, perp. to surface; includes sputtering from Mo spot and carbon surface.
[b] Average (and standard deviation) for probe-redeposited Mo ions.
[c] Average for Mo ions from ionization to probe redeposition.
[d] Including probe; essentially 100% redeposition.

velocity-changing collisions with the background plasma; with resulting spot-redeposition, on-probe non-spot redeposition and re-sputtering, and off-probe transport.

Table 1 summarizes several key simulation outputs. Among the major findings are a high spot redeposition fraction – particularly noteworthy considering the very small (1 cm) spot size – and high redeposition on the divertor generally, with little or no core plasma contamination (although a coupled WBC-plasma SOL code calculation would be needed to fully assess this).

Fig. 4 shows a code/data comparison of Mo areal density profile, at the end of the exposure. (The post-exposure spot areal density is based on the residual Mo depth, and assuming theoretical density). There is reasonable agreement, although with a higher predicted upstream transport of Mo than shown by the data. (Such discrepancy was also seen in an earlier experiment [7]).

The predicted Mo content in the carbon (Table 1) compares well with the measured value of 1.1×10^{16} atoms [6]. The simulation thus appears to completely explain the initially puzzling observation that only 19% of the Mo lost from the spot was seen in the probe carbon [6]. The reason is seen to be fast saturation of the Mo in C and subsequent re-sputtering, primarily to off-probe divertor areas. (For comparison, without a mixed-material effect – in particular with no re-sputtering of carbon-deposited Mo – 69% of spot-lost Mo is trapped in the carbon, or ~X5 higher than the reference case, and in major disagreement with the data).

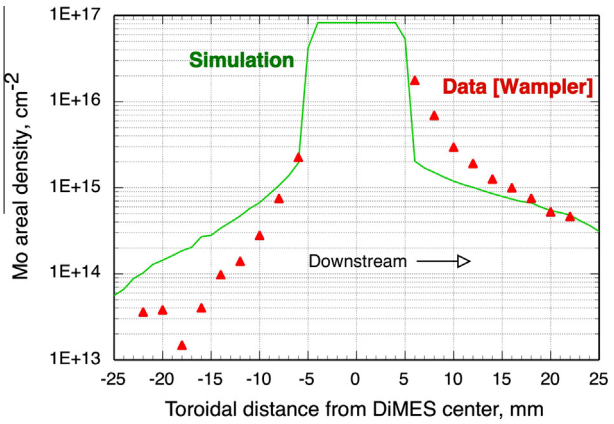

Fig. 4. Code/data comparison; Mo areal density along DIII-D toroidal direction, through probe center. Data from Ref. [6].

Another code/data check is as follows: The simulation computed gross erosion rate is ~1 nm/s, based on the input plasma parameters and computed particle fluxes and sputter yields. Using the 54% predicted redeposition rate then yields a net erosion rate of ~0.5 nm/s, again in good agreement with the measured value. Some additional code/data comparison issues are discussed further in Ref. [5].

Finally, simulations were run with variations in reference plasma conditions. Within the Te/Ne, etc., range explored, results are qualitatively similar. We do find, however, a high sensitivity of toroidal and radial Mo redeposition profiles to the azimuthal angle probability distributions for incident and sputtered particles. (The upstream/downstream transport code/data discrepancy could be due, in part, to this angular distribution sensitivity, issues with the background plasma specifications, and/or evolution of surface morphology at oblique angles. However, there is no obvious reason for the discrepancy identified, at this time).

3. Issues for ITER Be/W and NSTX Li/C/W mixing

The above results for Mo sputtering in DIII-D are favorable for ITER, implying high redeposition rates for the similar to Mo high-Z tungsten, and resulting low net erosion with negligible plasma contamination. A key issue, however, is the effect of the ~700 m^2 wall-sputtered Be on the ~50 m^2 W outer divertor, this potentially affecting Be/W alloy formation, thermal properties, divertor erosion, and T/Be codeposition in re-sputtered and off-divertor deposited Be. A previous study – using a simplified material response model – indicated no significant Be growth over most of the outer tungsten divertor, but with high Be growth at the strike point [1]. High-confidence, predictive ITER analysis can be performed with the advanced simulation method used here, however, the numerical issues become orders of magnitude greater. This is due to the ~50 cm long ITER divertor, with highly varying plasma parameters – compared to the 5 cm DiMES probe with near constant parameters. An added complication for ITER is the multiple particle impingement, due to D, T, He, and any trace impurity.

Likewise, the inner Mo divertor in NSTX-Upgrade will be subject to sputtered carbon transport from the first wall and lithium transport from other surfaces. A study using the present WBC/ITMC simulation method showed a complex evolution of the initially-Mo surface to one containing both Li, C and Mo, after only 1 s of NSTX plasma discharge, but this was only analyzed for a small area (at the strike point) [2]. As for ITER, a full mixed-material evolution study of a 15–30 cm wide NSTX Mo surface would require peta-scale computation.

4. Conclusions

It is clear that mixed-material plasma facing surface behavior is a key issue for fusion. We have described advanced modeling to study this, using coupled erosion/redeposition and material response code packages, with application to an important high-Z erosion/redeposition experiment in DIII-D. For DIII-D/DiMES, the simulation explains the important scientific result of high redeposition, quick saturation of sputtered/transported Mo in the surrounding C surface, and resulting transport to off-probe regions. The code/data match is generally good, but with a discrepancy in upstream/downstream transport. Resolving such discrepancy could be important for accurate determination of high-Z material net erosion rates, although the key picture of high redeposition somewhere on the divertor, and very low plasma contamination, would appear to be unaffected. For ITER, NSTX, and other large-area, low and high-Z mixed-material devices, our advanced analysis technique is highly applicable, but will require supercomputing.

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References

[1] J.N. Brooks, J.P. Allain, J. Nucl. Mater. 390–391 (2009) 123.
[2] J.N. Brooks, A. Hassanein, T. Sizyuk, J.P. Allain, "Modeling of plasma/lithium-surface interactions in NSTX: status and key issues", Fusion Engineering Design to be published.
[3] J.N. Brooks, Fusion Eng. Des. 60 (2002) 515.
[4] T. Sizyuk, A. Hassanein, J. Nucl. Mater. 404 (2010) 60.
[5] P.C. Stangeby et al., An experimental comparison of gross and net erosion of Mo in the DIII-D divertor, these proceedings.
[6] W.R. Wampler et al., Measurements of net erosion and redeposition of molybdenum in DIII-D, these proceedings.
[7] J.N. Brooks, D.G. Whyte, Nucl. Fusion 39 (1999) 525.
[8] J.N. Brooks, D. Najuoks, Phys. Plasmas 7 (2000) 2565.