Effect of surface segregation and mobility on erosion of plasma-facing materials in magnetic fusion systems

Tatyana Sizyuk and Ahmed Hassanein

Center for Materials Under Extreme Environment, School of Nuclear Engineering
Purdue University, West Lafayette, IN-47907, USA

The present work studies the combined effects of collisional sputtering and mixing processes of carbon impurities in tungsten plasma-facing material integrated with thermal processes including surface segregation and diffusion. We used our ITMC-DYN package, which includes description of all collisional and thermal processes, for the analysis of recent experimental results of tungsten erosion and carbon implantation at various target temperatures. Self-consistent integrated modeling predicted thermal processes effects on erosion/deposition dynamics and defined decisive parameters range and their importance. Critical parameters were estimated based on available experimental data. The integrated simulation reproduced the experimental results and predicted the transition from enhanced tungsten erosion to significant carbon coverage on the tungsten surface. These effects for wider range of system conditions with C/H ions irradiation and for reactor conditions can be predicted by including detailed modeling of chemical erosion processes in a self-consistent manner.

1. Introduction

Reliability and safety of magnetic fusion energy (MFE) devices will depend on stable operation and performance of plasma and lifetime of plasma-facing components (PFCs). Understanding plasma interaction with plasma facing surfaces in multicomponent environment is critical in assuring successful design and performance of a fusion reactor. This is because the interaction processes will affect the functional stability of PFCs and core plasma behavior, through fuel recycling and impurities accumulation. Prediction of materials erosion and dynamic

mixing and the subsequent changing of material properties during the long time of reactor operation is an important goal for the correct choice of materials. Recent work conducted in current tokamak reactors as well as ion beam sources and plasma wall interaction simulators are extensively used to benchmark the analysis of materials behavior at relevant conditions and in extrapolating the results to future reactor conditions.

Multiple beams, for example, consisting of hydrogen ions with various carbon concentrations to study impurity effects were used for analysis of tungsten samples heated up to 1000 K temperatures to simulate fusion environment [1]. It was found in these experiments that a small carbon content in ion beams, less than 1%, could accelerate blistering in tungsten. Modeling analysis using our ITMC-DYN computer simulation package has predicted that the formation of a carbon layer in tungsten sample with a relative concentration of carbon atoms above 50% significantly decreased hydrogen diffusion and desorption from the surface [2]. This leads to increased hydrogen accumulation near the surface and the subsequent diffusion to the bulk. Study of tungsten samples bombarded by deuterium with and without carbon inclusion indicated that carbon-seeded plasma extends temperature regime for blistering that can also be explained by the reduced mobility of deuterium even at relatively high temperatures [3]. Extensive studies of tungsten erosion due to carbon ions and simultaneous bombardment of deuterium and carbon were done for various sample temperatures [4-6]. These studies predicted the transition from extensive carbon covering of the surface at low temperatures to enhanced tungsten erosion at high temperatures. The analysis determined and highlighted several parameters that are important in understanding of C/W interactions, such as the importance of concentration-dependent carbon diffusion coefficient in tungsten and the chemical erosion yield at low target temperatures. These studies also highlighted the importance of accurate description and interplay

of several processes occurring on the surface during the deposition and interactions of ion beams with target material.

This paper presents results of our integrated modeling of tungsten surface evolution and erosion under bombardment by carbon impurities for reactor relevant temperatures regimes. We also analyzed the effect of various thermal processes at different temperatures based on several experimental results. Our Monte Carlo ITMC-DYN package [2, 7] was used for the self-consistent modeling of collisional mixing and interactions integrated with temperature dependent processes of particles diffusion and carbon impurity surface segregation. We further studied tungsten surface evolution when irradiated by carbon ions to determine the interplay of two possible processes in C/W compounds, such as diffusion and surface segregation, and to estimate parameters used in modeling of these processes.

We restrict our analysis in this paper only to C/W system, in particular to compare with recent experiments discussed above. However, the predicted effects can be extrapolated to the realistic reactor conditions based on the review and the simulation of other experimental results involving deuterium [5]. These experiments showed little influence of deuterium on tungsten sputtering and carbon deposition at elevated target temperatures considered in our analysis. It should also be mentioned that, while carbon is not currently considered as the main plasma-facing material for fusion reactor, it is interesting to understand recent experiments, especially since carbon is still used in current machines. In addition, carbon could be still interesting plasma-facing material due to the various current unresolved problems and issues associated with, e.g., the most promising full tungsten divertor material [8].

2. Surface segregation model integrated with other processes

The ITMC-DYN package is designed for simulation of material surface evolution due to ion beams irradiation. The package is based on Monte Carlo binary collision model integrated with models for various temperature-dependent processes such as particles diffusion, physical and chemical erosion, surface segregation, gaseous species molecular recombination, and desorption. Dynamic update of target composition takes into account the interaction of all above-mentioned time-dependent processes. The package includes several interatomic potentials for modeling of elastic atomic collisions and combination of several models for inelastic electronic energy loss. The collisional processes responsible for target atoms sputtering, mixing, and particles reflection are integrated self-consistently with time-dependent kinetic processes. Therefore, we can simulate the collisional and thermal processes occurring during beam/target interactions using actual experimental setup and conditions such as fluences and precise irradiation times and profiles of the experiments. Detailed description of models implemented in the ITMC-DYN package is given elsewhere [2, 7]. Below we briefly describe our surface segregation model since this is an important process in the present analysis of tungsten erosion under the impact of carbon impurity ions.

We used theoretical model for surface segregation described by du Plessis and van Wyk [9]. Their model is based on Darken's "uphill" diffusion and describes surface segregation as a diffusional process against the concentration gradient due to the difference in the chemical potential of the species from the surface to the bulk. The change in the chemical potential can be described for binary alloy as [9]:

$$\Delta G = \mu_1^B - \mu_1^S + \mu_2^S - \mu_2^B \quad (1)$$

where $\mu_1^B, \mu_2^B, \mu_1^S, \mu_2^S$ are the chemical potentials of species 1 and 2 in the bulk (B) and on the surface (S) respectively; ΔG is the change in Gibbs free energy. The segregation to the surface and particles motion in the bulk layers in binary alloys is given then by [9]:

$$\frac{\partial C_s(t)}{\partial t} = \frac{M_s}{a_1^2} C_1(t) \left[\Delta G + kT \ln \frac{C_1(t)(1 - C_s(t))}{C_s(t)(1 - C_1(t))} \right] \quad (2a)$$

$$\frac{\partial C_i(t)}{\partial t} = M_b kT \left[\frac{C_{i+1}(t)}{a_{i+1}^2} \ln \frac{C_{i+1}(t)(1 - C_i(t))}{C_i(t)(1 - C_{i+1}(t))} - \frac{C_i(t)}{a_i^2} \ln \frac{C_i(t)(1 - C_{i-1}(t))}{C_{i-1}(t)(1 - C_i(t))} \right] \quad (2b)$$

where C_s and C_i are the relative concentrations at the surface layer and at the i^{th} layer of the bulk respectively; a_i is the thickness of i^{th} layer; k is the Boltzmann's constant; T is the temperature; M_s and M_b are the mobility parameters of the species at the surface and in the bulk layers respectively which are related to the diffusion coefficient as [9]:

$$D = MkT \left(1 + \frac{\partial \ln f}{\partial \ln C} \right) \quad (3)$$

where f is the activity coefficient which indicates behavior of species in chemical compound. Since the activity coefficient is equal 1 in the case of ideal solution or constant in dilute solution, the last formula can be simplified to the following [9]:

$$M = \frac{D}{kT} \quad (4)$$

The main determining parameters in the surface segregation model described above are the difference in Gibbs free energy between the surface and the bulk, diffusion coefficients, and solution characteristics of formed compounds that determine the mobility of the species. We studied the range of validity and the accuracy of these parameters based on the extensive analysis of the experimental results during the interaction of carbon impurity ions with tungsten surfaces.

We also analyzed the difference in the bulk rate equations described by du Plessis (2b) and Fick's description of diffusion. We compared results produced by full du Plessis' description of surface segregation with results obtained by using Fick's model for the description of particles dynamics in the bulk layers integrated with du Plessis' model for the particles motion to the surface layer only, described by the equation (2a). Based on this comparison we found plausible relationship between the mobility parameter and the diffusion coefficient.

In summary, the main input parameters analyzed in this work were segregation energy, diffusion coefficient, and mobility coefficient. Our analysis was based on the review of the experimental data for two of these parameters, i.e., the diffusion coefficient [10] and the segregation energy [11]. The third parameter, the mobility of carbon to the surface layer, was estimated from our comprehensive simulations of several experiments. We evaluated possible variations of each of the above-mentioned parameters. The results show the overall effect of these variations on target evolution where the varied parameters are given in legends while the fixed parameters are included in figures captions. Other input parameters such as ion flux, ions energy, and angle of incidence in respect to the normal corresponded to the used parameters of the simulated experiments. Binding energies were fixed and corresponded to their conventional values.

3. Analysis of experimental results for C/W systems

The difference in Gibbs free energy, known as the segregation energy, depends on the temperature and elemental concentration of the compound. Experimental analysis of carbon segregation on tungsten surfaces showed that the segregation energy, while decreases with increasing the temperature and increases with increasing carbon loading in the samples, it

remains however of the order of 2 eV [11]. It was found in these experiments that little increase in carbon concentration in the target leads to an increase in both activation energies, i.e., for carbon transfer/migration from the surface monolayer into the bulk and for the escape/diffusion to the surface [11]. However, the transfer energy into the bulk becomes significantly higher that leads to the increase in the segregation energy, i.e., the difference between the above two activation energies. These variations are related to the carbides formation rates that are functions of temperature and carbon concentration [12]. Experiments also showed high rates of W_2C and WC formation at temperatures around 1000 K and higher [12]. It was also explained that changes in the diffusion coefficient of carbon due to increase of its concentration is related to the stoichiometry of carbides at corresponding temperatures [10].

We implemented in our package the parameters found in the experiments for the segregation energies [11] and for the diffusion coefficients [10, 13] to analyze and benchmark recent experimental data for tungsten erosion by carbon ions at different temperatures [5, 6, 14]. First, modeling of tungsten erosion and surface mixing was compared with experiments where tungsten samples were heated up to 970 K and then irradiated by 6 keV carbon ions with flux of $5 \times 10^{17} \text{ m}^{-2} \text{ s}^{-1}$ at 50 degree [14]. Figure 1 shows the steady-state carbon concentration on tungsten surface measured in the experiments and predicted by our ITMC-DYN package. Three important processes were analyzed in the modeling, i.e., target sputtering and mixing by collisional processes, carbon thermal diffusion, and carbon surface segregation. The surface binding energies used in the simulation, the main determining parameters influencing sputtering yields, were 8.68 eV for W and 7.4 eV for C. We implemented and analyzed various diffusion coefficients based on concentration-dependent values taken from [10] and possible increase of carbon diffusion due to irradiation [15]. Comparison of modeling results using several sets of the

diffusion coefficients is shown in Fig. 1. The maximum values of this parameter for low carbon concentration (< 0.2) were $4 \times 10^{-20} \text{ m}^2 \text{ s}^{-1}$ and $8 \times 10^{-20} \text{ m}^2 \text{ s}^{-1}$ that correspond to values found in different experiments for similar temperature [10, 13]. We varied the highest and the lowest diffusion coefficients to estimate effect of concentration-dependent coefficients at the considered temperatures (Fig. 1) and to predict the range of effective diffusion coefficients for lower target temperatures at the given irradiation conditions. We used in our modeling an average energy for carbon segregation on tungsten surface of about 2 eV [11] and $5 \times 10^{-22} \text{ m}^2 \text{ s}^{-1} / kT$ for the mobility coefficient on the surface (M_s) that is significantly lower than possible mobility of carbon in ideal or dilute solution based on the diffusion coefficients considered above (Eq. 4). The high probability of W_2C and WC formation at the considered 970 K temperature [12] results in stronger bonds in the formed compound. This can significantly decrease atoms mobility that affects carbon segregation to the surface. At the same time, the high sputtering yield of tungsten and carbon at 50° angle of ions incidence (in respect to the normal), around 0.8, results in high erosion rate of the target. This prevents covering of the surface by carbon and overall reduces the effect of target temperature on the erosion processes for the ion parameters considered in this analysis. These experiments showed that the steady-state carbon concentration in the target was approximately the same at 300 K and 970 K temperatures [14]. The slight increase in carbon concentration on the surface with higher temperature can be due to carbon segregation to the surface during irradiation as seen in Fig. 1. Further diffusion and surface segregation after the irradiation could be the reason for the differences in modeling and experimental results.

Fig. 1. Steady-state carbon concentration on the tungsten surface due to 6 keV carbon ions irradiation with $5 \times 10^{17} \text{ m}^{-2} \text{ s}^{-1}$ intensity at 50° of incidence angle (used parameters for surface segregation: $\Delta G = 2 \text{ eV}$; $M_s = 5 \times 10^{-22} \text{ m}^2 \text{ s}^{-1} / \text{kT}$)

This situation changes if the bombarding ions with the same energy have smaller angle of incidence of 15° to the normal [6]. The more than two times reduction in the sputtering yield of carbon resulted in the accumulation of carbon on tungsten surface at 300 K temperature. This resulted in carbon to fully cover the surface after certain time (Fig. 2), which was indicated by the termination of tungsten erosion shown in Fig. 3. The calculated carbon implantation, the difference between incoming carbon (dotted black line) and sputtered and reflected, is shown in Fig. 2 as a function of fluence. At higher, 870 K target temperature however, carbon coverage of the surface was significantly delayed and an increased tungsten erosion was found (Figs. 2, 3).

Fig. 2. Carbon implantation at 300 K and 870 K. Ion beam parameters: $10^{18} \text{ m}^{-2} \text{ s}^{-1}$, 6 keV at 15° of incidence. Modeling of diffusion and surface segregation at 870K: $\Delta G = 2 \text{ eV}$; $D = 7 \times 10^{-20} \text{ m}^2 \text{ s}^{-1}$; $M_s = 10^{-21} \text{ m}^2 \text{ s}^{-1} / kT$

Fig. 3. Tungsten erosion by carbon ions at 300 K and 870 K. Ion beam parameters: $10^{18} \text{ m}^{-2} \text{ s}^{-1}$, 6 keV at 15° of incidence. Modeling of diffusion and surface segregation at 870K: $\Delta G = 2 \text{ eV}$; $D = 7 \times 10^{-20} \text{ m}^2 \text{ s}^{-1}$; $M_s = 10^{-21} \text{ m}^2 \text{ s}^{-1} / kT$

Several processes can cause enhanced sputtering of tungsten and carbon at higher temperatures. First, radiation enhanced diffusion (RED) due to high radiation damage in tungsten by the energetic 6 keV ions can be significant at the considered temperature, and become much higher than pure thermal diffusion [15]. The RED increases and promotes the transfer/migration of carbon atoms from the main deposition area to the surface as well as to the bulk. Second, carbon segregation to the near surface layers further increases carbon motion/diffusion to the surface. Combination of these processes results in accumulation of carbon on the surface that leads to higher carbon sputtering by the incoming ions. Migration of carbon to the surface and the subsequent increase in sputtering, however, reduces its accumulation in the target. As a result, the more collisions of ions with tungsten atoms also lead to the enhanced erosion of tungsten.

ITMC-DYN simulation results were obtained integrating collisional and thermal processes described above. Carbide crystallite formation and lateral inhomogeneity in the target may affect

the sputtering/deposition processes. Modeling of ions/target interaction taking into account lateral inhomogeneity requires parallel simulations as well as implementation of models for the description of possible inhomogeneity. We did not consider this effect in the current simulation. However, it would not change the general dynamics of all processes. Energetic ions will cause many collisions in the target that will lead to intense carbon redistribution and will quickly change surface morphology to amorphous like structure, i.e., reducing lateral inhomogeneity effects during irradiation. Results shown in Figs. 2, 3 are in good agreement with experimental measurements except the data for carbon implantation at higher fluence in the target at 870 K. The linear increase in carbon implantation at fluence $> 2.5 \times 10^{22} \text{ m}^{-2}$ indicates that the surface was covered by carbon and incoming ions interacted only with carbon atoms. Therefore, modeling results at this time were determined only by collisional processes, which were similar to 300 K case. Further detailed analysis, both experimental and modeling, is required to find possible reasons of the difference in carbon self-sputtering at various temperatures found in these experiments [6].

Fig. 4. Carbon concentration on the surface due to 10^{21} m^{-2} fluence. Ion beam parameters: $10^{18} \text{ m}^{-2} \text{ s}^{-1}$, 6 keV at 15° of incidence. Modeling of diffusion and surface segregation at 870K: $\Delta G = 2 \text{ eV}$; $D = 7 \times 10^{-20} \text{ m}^2 \text{ s}^{-1}$; $M_s = 10^{-21} \text{ m}^2 \text{ s}^{-1} / kT$

Fig. 5. Carbon concentration on the surface due to $5 \times 10^{21} \text{ m}^{-2}$ fluence. Ion beam parameters: $10^{18} \text{ m}^{-2} \text{ s}^{-1}$, 6 keV at 15° of incidence. Modeling of diffusion and surface segregation at 870K: $\Delta G = 2 \text{ eV}$; $D = 7 \times 10^{-20} \text{ m}^2 \text{ s}^{-1}$; $M_s = 10^{-21} \text{ m}^2 \text{ s}^{-1} / kT$

Figures 4 and 5 show the difference in target evolution and carbon buildup for two different temperatures predicted in our modeling. Carbon concentration is almost the same at RT and at 870 K temperature after irradiation of 10^{21} m^{-2} fluence (Fig. 4). Results in Fig. 4 reflect mostly the collisional processes of carbon ions with tungsten with 10 nm implantation range for the considered ion energy. The erosion rates for both temperatures were the same (Figs. 2, 3). At later times, the increased carbon accumulation on the surface at 300 K significantly reduced tungsten sputtering. Longer ions range in the formed compound, around 15 nm, further affected the buildup of carbon layer (Fig. 5). At higher target temperature, carbon diffusion and segregation to the surface increased tungsten sputtering rates and delayed carbon accumulation in the target. The results shown in Figs. 4 and 5 for 870 K were obtained using the diffusion coefficient of $7 \times 10^{-20} \text{ m}^2 \text{ s}^{-1}$, the segregation energy of 2 eV, and the mobility coefficient on the surface of $10^{-21} \text{ m}^2 \text{ s}^{-1} / kT$. The last parameter is higher than for 970 K due to the difference in compounds formation that can significantly affect the mobility of carbon.

Self-consistent simulation of target response at higher temperature requires comprehensive understanding of several parameters and coefficients. It is quite a challenging task to accommodate all parameters involved in the simulation of complex set of processes in continuously evolving system. However, we found several dependencies that allowed us to correctly reproduce the experimental results. Our analysis was based on the values predicted in various experiments [11, 13].

First, we analyzed the effect of diffusion coefficient of carbon on tungsten erosion. Enhanced carbon diffusion due to high diffusion of vacancies from the main damaged region was also taken into account. Based on this we found that the diffusion coefficient in the main deposition region can vary from around $5 \times 10^{-20} \text{ m}^2 \text{ s}^{-1}$ to $10^{-19} \text{ m}^2 \text{ s}^{-1}$ as shown in Fig. 6. Lower diffusion

coefficients lead to higher carbon sputtering at earlier time, due to higher carbon concentration in the ions range area, and to the faster carbon buildup at later time which results in the reduction of tungsten sputtering (Fig. 7). Higher diffusion coefficients lead to higher tungsten erosion. The overall transition between enhanced target erosion and carbon layer buildup is determined by the relation between carbon transferred to bulk due to collisions and diffusion and carbon transferred to surface layers by diffusion and surface segregation.

Fig. 6. Effect of diffusion coefficient on carbon implantation at 870 K ($\Delta G = 2$ eV; $M_s = 10^{-21} \text{ m}^2 \text{ s}^{-1} / kT$)

Fig. 7. Effect of diffusion coefficient on tungsten sputtering at 870 K ($\Delta G = 2$ eV; $M_s = 10^{-21} \text{ m}^2 \text{ s}^{-1} / kT$)

Two parameters are needed to model surface segregation, i.e., the segregation energy and the mobility coefficient. The mobility coefficient is related to the diffusion coefficient and depends on chemical compound (Eq. 3). Moreover, atoms transfer to the surface layer can be much slower than the supply of atoms from the bulk to the near surface layer according to [9], therefore the mobility parameter for the surface can be much smaller than for the bulk. To estimate the relation between the mobility coefficient and the diffusion coefficient we analyzed two models for the simulation of carbon dynamics in the bulk, Fick's diffusion and de Plessis rate equation for the bulk. The latter method produces the same to Fick's diffusion results based

on several assumptions [16]. Figure 8 shows that both models produce similar results with the assumption of the reduced mobility parameter that corresponds to non-dilute and non-ideal compounds (Eq. 3). We used different mobility parameters for the simulation of carbon dynamics in the bulk, M_b (given in Fig. 8 legend) and carbon segregation to the surface layer, M_s (given in Fig. 8 caption). The last one was further reduced that allowed reproducing experimental results based on the real measurable value such as the segregation energy [11].

Fig. 8. Relation between the diffusion coefficient (Fick's model) and the mobility parameter for the bulk (Darken modified by de Plessis) ($\Delta G = 2$ eV; $M_s = 10^{-21} \text{ m}^2 \text{ s}^{-1} / kT$)

An average energy for carbon segregation was measured around 2 eV. We analyzed the effect of the segregation energy on the resulting erosion and deposition processes. Figures 9 and 10 show that changes in the segregation energy did not influence much the carbon implantation at earlier time, i.e., lower fluences. However, lower value of the segregation energy leads to faster carbon accumulation near the surface that reduced tungsten erosion as shown in Fig. 10.

Fig. 9. Effect of the segregation energy on carbon implantation at 870 K ($D = 7 \times 10^{-20} \text{ m}^2 \text{ s}^{-1}$; $M_s = 10^{-21} \text{ m}^2 \text{ s}^{-1} / \text{kT}$)

Fig. 10. Effect of the segregation energy on tungsten sputtering at 870 K ($D = 7 \times 10^{-20} \text{ m}^2 \text{ s}^{-1}$; $M_s = 10^{-21} \text{ m}^2 \text{ s}^{-1} / \text{kT}$)

Possible uncertain dependencies can be in the combination of both the segregation energy and the mobility coefficient for the surface. Reducing one value requires increasing the other one. However, these parameters should be around the experimental average value for the segregation energy, which is a measurable value.

Fig. 11. Effect of the mobility coefficient on carbon implantation at 770 K ($\Delta G = 2 \text{ eV}$; $D = 4 \times 10^{-20} \text{ m}^2 \text{ s}^{-1}$)

Fig. 12. Effect of the mobility coefficient on tungsten sputtering at 770 K ($\Delta G = 2 \text{ eV}$; $D = 4 \times 10^{-20} \text{ m}^2 \text{ s}^{-1}$)

To demonstrate the viability of our approach and the validity of the above-described methods for the analysis of such processes at other target temperatures, we simulated the experiments with target performed at 770 K temperature [6]. Figures 11 and 12 show the effect of the mobility coefficient at the surface with fixed, 2 eV value of the segregation energy and $4 \times 10^{-20} \text{ m}^2 \text{ s}^{-1}$ for the diffusion coefficient. The diffusion coefficient used was higher than found in the experiments for this temperature [13] to take into account RED. The probability of carbides formation at this target temperature is similar to 870 K [12]. Therefore, we again related the mobility coefficient at the surface with the diffusion coefficient in the target in similar way that is reduced by two orders of magnitude in comparison with ideal or dilute alloys. Figures 11 and 12 demonstrate the logic and feasibility behind this relationship. Using the same values of the segregation energy and the same relationship between the diffusion coefficient and the mobility parameter, and conserving all other input parameters, we reproduced the experimental results for different target temperatures.

Fig. 13. Dependence of tungsten erosion on ion flux at 870 K ($\Delta G = 2 \text{ eV}$; $D = 7 \times 10^{-20} \text{ m}^2 \text{ s}^{-1}$; $M_s = 10^{-21} \text{ m}^2 \text{ s}^{-1} / \text{kT}$)

Fig. 14. Dependence of W erosion / C implantation on C content in beam with D ions at 870 K ($\Delta G = 2 \text{ eV}$; $D = 7 \times 10^{-20} \text{ m}^2 \text{ s}^{-1}$; $M_s = 10^{-21} \text{ m}^2 \text{ s}^{-1} / \text{kT}$)

The effect of thermal processes on target erosion can also be verified by comparing the results obtained with different fluxes. Figure 13 shows that ten times decrease in ions flux leads to the transition from the increased carbon accumulation and reduced tungsten sputtering by $5 \times 10^{18} \text{ m}^{-2} \text{ s}^{-1}$ ion flux to the continuous tungsten erosion by $5 \times 10^{17} \text{ m}^{-2} \text{ s}^{-1}$ flux.

The above results for the flux-dependence can be also useful for the prediction of considered effects in the experiments with mixed ion beams including hydrogen isotopes. Experimental results with different carbon content in ion beam showed that processes of W sputtering and C implantation at the elevated temperatures are determined mainly by carbon influx [5]. Fig. 14 shows relation between sputtered W and implanted C for several ion beam compositions. In this simulation, we used parameters relevant to these experiments [5] such as 6 keV C and 3 keV D ions at 15° angle of incidence with respect to the normal with D flux of 10^{18} – 10^{19} ions/ $\text{m}^2 \text{ s}$ and C flux of 7×10^{17} ions/ $\text{m}^2 \text{ s}$ in ion beam with 7% of carbon and 10^{18} ions/ $\text{m}^2 \text{ s}$ in other cases. Beams with low C influx, with or without D inclusion (Figs. 13 and 14), lead to continuous tungsten erosion and steady-state carbon concentration. Addition of D ions with relatively high energy increases erosion of both W and C that can be seen from comparative analysis of results for 25% and 100% C concentrations in ion beam (Fig.14). These results were produced without modeling of chemical erosion. Good agreement of simulation results with measurements illustrates the small effect of chemical erosion for the resulted concentrations of carbon in the target due to the high diffusion of hydrogen to the bulk at the considered temperature [17, 18].

Ions flux, energies, composition, and angle of incidence should be further analyzed to find the exact dependences and interplay of these physical processes in overall dynamics of surface evolution in mixed materials environment in future MFE devices.

4. Conclusion

We developed and implemented models in our ITMC-DYN Monte Carlo simulation package to study mixing materials evolution and resulting effects on plasma performance and erosion lifetime of MFE-related materials. We combined and integrated collisional and thermal processes to study tungsten erosion by the energetic carbon impurity ions during plasma operation. Integrated self-consistent simulation of particles collisional processes, radiation enhanced diffusion, and surface segregation allowed explaining recent experimental results regarding the difference in tungsten erosion and buildup of carbon layer at different target temperatures. Based on various experimental predictions for the diffusion coefficients and the segregation energy we found several key dependences that can affect carbon impurity behavior in tungsten at various temperatures. The integrated simulation allowed reproducing the experimental results and predicting transition from enhanced tungsten erosion to significant surface coverage by carbon on the tungsten surface. Simulations for wider range of system conditions including mixed ion beams with hydrogen isotopes content can be done by including detailed modeling of chemical erosion in self-consistent analysis. The developed models and simulation package can then be used to predict mixed materials behavior and evolution and the effect on plasma operation in future devices such as ITER.

Acknowledgment

This work is partially supported by the US DOE, Office of Fusion Energy Sciences, and the National Science Foundation (PIRE) project.

References

1. Y. Ueda, T. Shimada, and M. Nishikawa, Nucl. Fusion 44 (2004) 62.
2. T. Sizyuk, A. Hassanein, J. Nucl. Mater. 404 (2010) 60.

3. V. Kh. Alimov, J. Roth, R. A. Causey, D. A. Komarov, Ch. Linsmeier, A. Wiltner, F. Kost, S. Lindig, J. Nucl. Mater. 375 (2008) 192.
4. K. Schmid, J. Roth, J. Nucl. Mater. 313–316 (2003) 302.
5. H. T. Lee, K. Krieger, J. Nucl. Mater. 390–391 (2009) 971.
6. H. T. Lee and K. Krieger, Phys. Scr. T138 (2009) 014045.
7. A. Hassanein and D. L. Smith, Nucl. Instr. and Meth. B 13 (1986) 225.
8. T. Tanabe, Phys. Scr. T159 (2014) 014044.
9. J. du Plessis and G. N. van Wyk, J. Phys. Chem. Solids 50 (1989) 237.
10. K. Schmid, J. Roth, J. Nucl. Mater. 302 (2002) 96.
11. N. D. Potekhina, N. R. Gall', E. V. Rut'kov, and A. Ya. Tontegode, Phys. Solid State 45 (N4) (2003) 782.
12. J. Luthin, Ch. Linsmeier, Surface Science 454–456 (2000) 78.
13. K. Schmid, J. Roth, W. Eckstein, J. Nucl. Mater. 290-293 (2001) 148.
14. I. A. Bizyukov, J. W. Davis, A. A. Haasz, P. Brodersen, J. Nucl. Mater. 400 (2010) 245.
15. G. S. Was, Fundamentals of Radiation Materials Science, Springer Berlin Heidelberg, New York, 2007.
16. J. du Plessis and E. Taglauer, Surface Science 260 (1992) 355.
17. W. Wang, V.Kh. Alimov, B.M.U. Scherzer, J. Roth, J. Nucl. Mater. 241-243 (1997) 1087.
18. V.Kh. Alimov, J. Roth, R.A. Causey, D.A. Komarov, Ch. Linsmeier, A. Wiltner, F. Kost, S. Lindig, J. Nucl. Mater. 375 (2008) 192.

- We integrated collisional and thermal processes to study tungsten erosion by carbon ions.
- We analyzed effects of radiation enhanced diffusion and surface segregation.
- Self-consistent simulations allowed explaining experimental results.
- Difference in tungsten erosion at various temperatures was explained.