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

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HIGHLIGHTS

- 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.

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ABSTRACT

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

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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]:

$$\Delta G = \mu_1^B - \mu_1^S + \mu_2^S - \mu_2^B \tag{1}$$

where μ_1^B, μ_2^B, μ_1^S, μ_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]:

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

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

where C_s and C_i are the relative concentrations at the surface layer and at the ith layer of the bulk respectively; a_i is the thickness of ith 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]:

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

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]:

$$M = \frac{D}{kT} \tag{4}$$

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's 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's model for the particles motion to the surface layer only, described by Eq. (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.