Dynamic Simulation of Materials Modification and Deuterium Retention in Tokamak Fusion Environment

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ABSTRACT

The ability of plasma-facing materials (PFM) in fusion reactor to withstand subsequent erosion as well as deuterium and tritium accumulation depends on material properties, which will continuously be changed during reactor operation. Variation in plasma parameters, using various materials for coating of reactor walls, e.g., Be for the first wall and W and C for the divertor area, and the presence of gases/impurities in the chamber will result in subsequent PFMs surface modification that will seriously affect deuterium/tritium retention and recycling as well as plasma operation. We modeled tungsten surface evolution during reactor operation for ITER relevant parameters of ions energy, fluence, and composition. We used our ITMC-DYN Monte Carlo package for the self-consistent integrated simulation to predict the effect of edge plasma conditions and impurities concentration on deuterium deposition, diffusion, and trapping. Processes of ions/target interaction, physical and chemical erosion, particles diffusion, molecular recombination and desorption were benchmarked with recent experimental results. Relation between ions fluence and blistering in near-surface layers was studied. A study was also performed for carbon co-deposition as an enhancing factor for tungsten erosion and blistering. Implementation of surface segregation and particles diffusion in composite materials allowed correct understanding of surface evolution at different target temperatures.

KEYWORDS: Plasma-Facing Materials, Hydrogen Retention, Erosion, ITMC-DYN

1. INTRODUCTION

Reliable and safe operation of future fusion energy devices depends on many factors where consequences of plasma/wall interactions can be considered as the most important area for research and development. Plasma energy and particles deposition on surfaces of reactor walls; energetic runaway electrons and neutrons penetration; hydrogen isotopes diffusion and retention; and plasma energy transfer to deeper layers of plasma facing components (PFC) will cause materials erosion and damage that significantly change initial materials properties and by-turn will influence reactor environment and plasma performance. In this regard, mixing and degradation of materials at the surface layers will play significant role on reactor operation since these processes will continuously occur at the steady-state regime and they will determine important parameters such as fuel recycling.

For example, complex structure of the divertor in ITER design with carbon and tungsten surfaces on inner and outer vertical targets, beryllium walls, and presence of gases in chamber will lead to mixed materials formation and significant changes in the properties of plasma facing materials. Extensive experimental research as well modeling analysis is being conducted for prediction of materials mixing and performance at different ITER relevant conditions. These studies showed that slight variations in parameters or conditions of experimental environment could significantly change deuterium diffusion and recycling, influence materials modification. These showed also the necessity of the self-consistent integrated modeling of all important processes occurring during ions/target interactions.

Dynamic tracking of surface evolution at nano/micro layers subjected to various plasma species was performed using Monte Carlo binary collision

approximation models that include most important processes of ions/atoms interactions and time-dependent evolution of target composition. We studied various parameters that influence materials erosion and modification, hydrogen isotopes recycling and bulk penetration.

2. SELF-CONSISTENT SIMULATIONS OF IONS/TARGET INTERACTIONS

The dynamic version of ITMC [1] (Ion Transport in Materials and Compounds), i.e., ITMC-DYN code [2] includes several implemented interatomic potentials for modeling of elastic atomic collisions; combination of several models for inelastic electronic energy loss; dynamic time-dependent update of target composition; implanted atoms diffusion and mixing; molecular surface recombination and desorption; chemical erosion, and surface segregation. The ion–atom and atom–atom elastic interactions are modeled based on the common form of a screened Coulomb potential between the interacting species. Three screening functions are implemented in ITMC-DYN code: Moliere, KrC, and ZBL. The electronic energy losses are described in the code by two methods: combination of the Lindhard–Scharff–Schiott (LSS) and Bethe models and using Ziegler fitting coefficients. The collision processes responsible for target atoms sputtering, mixing and particles reflection are integrated with detailed models of time-dependent atoms diffusion, surface segregation and molecular recombination and desorption. Therefore, we considered actual fluences and exact irradiation times. Descriptions of all processes shown in **Figure 1** are integrated in the package in self-consistent matter that allows modeling of realistic experimental conditions and parameters and predict various phenomena.

Detail description of models and approaches implemented in the ITMC-DYN package is given in [2].

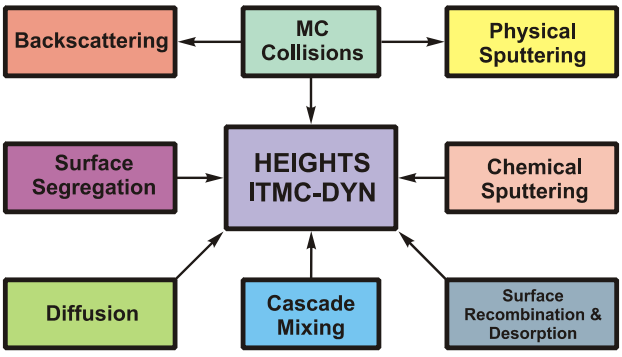

Fig. 1 Integrated modeling in ITMC-DYN package.

3. RESULTS AND DISCUSSION

3.1 Hydrogen isotopes diffusion in mixed materials

Clean tungsten plasma facing materials have low solubility and high diffusion of hydrogen isotopes and will result in high recycling of hydrogen. Retention in bulk tungsten will be controlled only by defects such as intrinsic lattice imperfections and neutron induced damage. However, tungsten surfaces in the divertor area are subjected to intense bombardment of plasma ions mixed with impurities, such as carbon, oxygen, and/or beryllium, which can lead to significant changes in hydrogen diffusion, retention and recycling. **Figure 2** illustrates the large difference in hydrogen diffusion in pure tungsten [3] and in randomly oriented carbon [4].

Several parameters can influence hydrogen behaviour including particle fluence, surface temperature, impurities content and concentration. We simulated set of experiments related to the ITER environment where mixed beam of hydrogen and carbon ions bombarded tungsten samples [5]. The incident ion beams consisted of 70% of 333 eV H^+, 10% of 500 eV H^+, 20% of 1000 eV H^+ and from 0.1% to 1.5% of C ions with 1000 eV. Varying ions fluence, concentration of hydrogen and carbon in ions beam, and samples temperature, conditions for blistering formation in tungsten were found. We considered these experiments for benchmarking of our models and for analysis of processes that might influence hydrogen accumulation and blistering [2],[6]. **Figure 3** shows modeling results for deposited carbon concentration on W surface in dependence on carbon concentration in ions beam. It illustrates that minute changes in C ions concentration significantly influences carbon layer formation and,

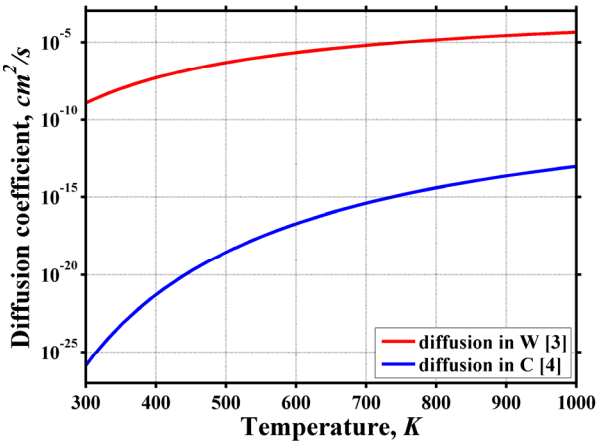

Fig. 2 Diffusion coefficients of hydrogen isotopes in tungsten and in carbon.

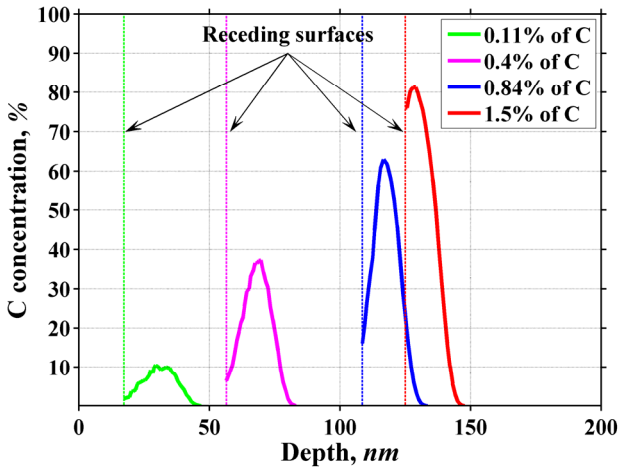

Fig. 3 Concentration of C in tungsten at temperature 653 K and fluence of 3 x 10^{20} H/cm^2 with 0.11%, 0.4%, 0.84%, and 1.5% of C in ion beam.

as it will be shown later, hydrogen diffusion and retention.

It was shown in the experiments that an increase of carbon in ions beam to 0.8%, leads to blisters formation in the near-surface layers of W samples. We studied the mechanisms that could cause hydrogen accumulation in samples and resulting blistering.

Deposition of carbon layer on tungsten, in the form of graphite or in binding with tungsten (WC or W_2C) on the surface of the samples [7], influenced hydrogen diffusion to the bulk and to the surface and subsequent molecular recombination and desorption from the surface. Using experimental results for hydrogen isotopes diffusion in tungsten and in carbon, we calculated the diffusion coefficient in multi-component materials depending on target composition as the interpolation of logarithmic values of diffusivity in each compound. **Figure 4** shows that hydrogen concentration is significantly increased in the layer of deposited carbon. It is also shown in the figure that for larger carbon inclusion in ions beam, 0.8% and more, carbon layer acts as barrier for hydrogen diffusion to the surface reducing probability of molecular recombination and desorption.

It was found in the experiments that blisters appear at higher fluences of ions, more than 10^{19} H/cm^2. **Figure 5** shows dependence of hydrogen accumulation on the surface on the ions fluence. Ions flux used in these simulations was the same as in the experiments.

Thus, minute inclusion of carbon in ion beam causes hydrogen accumulation in tungsten that leads to following blistering and material degradation.

3.2 Influence of impurities on target material mixing and erosion

Concentration of carbon in ions beam determines also target erosion and carbon concentration profile. Carbon profiles are shown relatively to the initial position of tungsten surface. In the cases of higher carbon content in the ions beam erosion of samples was around 100 nm and more. Our modeling predicted samples erosion that is comparable with those found in the experiments [8]. Figure 3 also shows that beams with lower carbon concentration produced broader profiles. This is

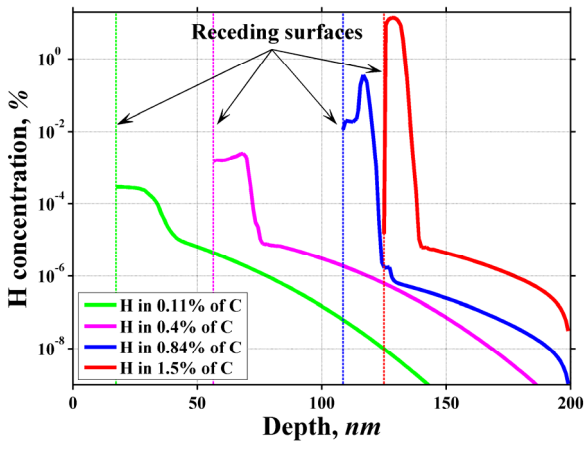

Fig. 4 Accumulation of H in tungsten at temperature 653 K for flux of 3 x 10^{17} H/cm^2/s and fluence of 3 x 10^{20} H/cm^2 with 0.11%, 0.4%, 0.84%, and 1.5% of C in ion beam.

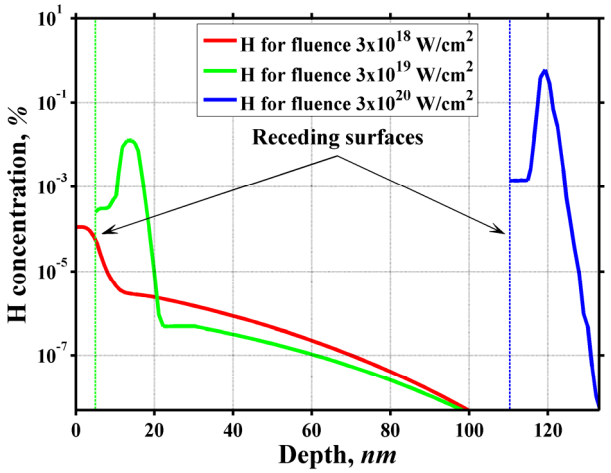

Fig. 5 Accumulation of H in tungsten at temperature 653 K for flux of 3 x 10^{16} H/cm^2/s and different fluences with 0.84% of C in ion beam.

explained by differences in the target erosion. Carbon atoms, redistributed inside the W target by incoming hydrogen ions are then removed by surface erosion and this process is accelerated in the case of 0.84% C concentration in the beam.

The difference in our modeling and in experiments was related to the peak location of carbon profile. Experimental results showed the peak closer to the surface. To analyze this difference we considered two additional and important processes, i.e., surface segregation and samples etching by Ar ions since the concentration profiles in the experiments were found using the XPS sputter technique utilizing 1.7 keV Ar ions.

The process of surface segregation moves carbon atoms from the bulk to the surface layer because of the increase in the chemical potential of carbon in the bulk of W/C compound [2]. Modeling of this phenomenon can shift the peak of the carbon concentration profile to the surface. However if we consider this process self-consistently with ions beam deposition, target atoms sputtering, and atom cascade mixing/redistribution, the effect of surface segregation loses its effectiveness. The segregated carbon atoms moving to the surface will be knocked out by the incident ions beam.

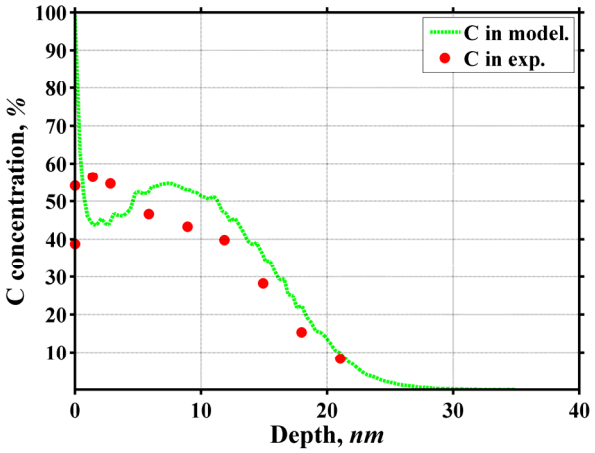

Fig. 6 Concentration of C in tungsten sample after deposition of H with 0.8% C in total fluence of $3x10^{20}$ H/cm^2 and sample temperature of 653 K. Modeling included also post-irradiation surface-segregation and etching by 1.7 keV Ar ions.

Surface segregation is a time-dependent process and can take a place during post-irradiation period. Carbon concentration increase on the surface is significant during this time and we analyzed the influence of this surface segregation process as well etching on the resulting concentration profile. **Figure 6** shows comparison of the resulting carbon profile after the inclusion of all above listed processes with the profile obtained in the experiments. Better agreement of modeling results with experimental data was obtained at higher irradiation temperatures [2].

4. CONCLUSION

Utilizing our dynamic Monte Carlo package, ITMC-DYN, we identified, modeled, and analyzed important processes occurring during ions/target interaction for ITER relevant parameters and materials. Self-consistent implementation of all processes involved in modeling material evolution during ions beam bombardment is very important in understanding dynamics of surface erosion, mixed materials evolution, and hydrogen isotope behavior and retention in materials. Modeling analysis showed that minute inclusion of impurities during ion beam irradiation, e.g., carbon content of less than 1%, can significantly influence materials surface mixing, material erosion, hydrogen diffusion, and retention.

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