Dynamic analysis of mixed ion beams/materials effects on the performance of ITER-like devices

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ABSTRACT

Future reactors, e.g., ITER can require multiple plasma facing components (PFC) surfaces such as Be, C and W. Soon after the start of normal operation as well as after plasma transient events the surfaces can behave much differently than the original surfaces, and transport of eroded particles can influence plasma performance and component lifetime.

A new dynamic version of ITMC-DYN, part of the HEIGHTS package, is therefore developed for detailed investigation of plasma material interaction in multiple/mixed materials environment. Models consider simultaneous ion penetration and mixing, scattering, reflection, physical and chemical sputtering, dynamic surface evolution/modification, thermal diffusion, hydrogen molecular recombination, and surface segregation. The package tracks time and temperature-dependent dynamic changes in surface erosion/growth rate, and material composition and structure. Initial results show significant influence of mixed beams/materials on PFC erosion, material evolution, hydrogen isotope behavior, and potential plasma performance. We analyzed recent experiments on hydrogen isotope retention in ITER relevant mixed materials, and predict the behavior of hydrogen (retention, diffusion, molecular recombination, and blister formation). Excellent code/data agreement is obtained and conditions of blister formation are identified and explained.

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1. Introduction

Composite/mixed materials as plasma facing components (PFC) in, e.g., ITER add complexity to understanding the effects of core plasma particles impact on PFC surface, erosion lifetime, core plasma contamination, fuel particle recycling, and coating material protective properties. For example, impingement of hydrogen isotopes and helium ions from the core plasma with impurities of beryllium and carbon eroded from PFC can cause erosion, sputtering, and chemical interactions with a tungsten divertor surface, for example, that will result in mixed layers of materials, possible compound formation, and changing of surface thermodynamic and mechanical properties that will impact materials performance and lifetime.

In the case of hydrogen ion interactions with solid tungsten surface, the ion deposition mainly leads to ion reflection/backscattering from the surface, molecular recombination and thermal desorption from the surface layers, physical sputtering of target atoms, and possible bubble formation and structural changes. The latter three processes depend on ion energy, fluence, and target temperature as well as on materials properties. Hydrogen diffusion in tungsten is high for ITER relevant temperatures – operating temperatures around 1000 K can be achieved – and hydrogen isotope retention is low in pure tungsten. Hydrogen trapping can result from intrinsic traps in imperfect lattices or ion-induced traps; this increases with increasing ion energy and fluence. Irradiating tungsten using pure hydrogen isotope beams in laboratory experiment may not be sufficient to understand the behavior in tokamak reactors. An enhanced erosion of W coating by core plasma ions can occur due to the presence of minute impurities like carbon, oxygen, or beryllium. These impurities will also influence hydrogen retention processes since traps produced by heavier ions will increase and the formation of composite materials will significantly affect surface hydrogen molecular recombination and retention, chemical bonding with target atoms, and the mobility of the incident ions.

Comprehensive experiments were recently conducted to investigate surface erosion, impurity material deposition and concentration, and blister formation in tungsten under the impact of hydrogen ion beams with embedded carbon impurities [4,8]. The dependence of material erosion and blister formation on incident ion fluence with various carbon concentrations at different target temperatures was studied.

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material interaction of multiple incident ion beams in mixed materials environment. We modeled these experiments, in detail, to benchmark our enhanced ITMC-DYN code and to predict the behavior of PFC in real reactor environment. We implemented simultaneous multiple incident ion beams deposition having different energies and included self-consistently the time-dependent processes of diffusion, segregation, and surface recombination.

We have studied both the influence of such processes occurring at the time of the beam deposition as well as post-irradiation processes during sample analysis including diffusion, carbon surface segregation, and etching by Ar ions. Our results showed the importance of the self-consistent integrated modeling of all above-mentioned processes in understanding material erosion and lifetime and conditions for blister formation that can be serious obstacle of the potential use of tungsten as plasma facing material.

2. Brief description of ITMC-DYN integrated models

The Monte Carlo based Ion Transport in Materials and Compounds (ITMC) code [1–3] has been significantly enhanced and now includes the following capabilities: (1) implementation of screening functions such as ZBL, KrC, or Molière for the Coulomb potentials in modeling elastic atomic collisions; (2) implementation of combination of LSS and Bethe models and Ziegler fitting coefficients for the inelastic electronic energy loss; (3) dynamic update of target composition; (4) unlimited number of target layers with unlimited number of composite materials; (5) unlimited number of incident simultaneous ion beams with different parameters; (6) implanted atoms diffusion and mixing; (7) molecular surface recombination and desorption; (8) physical and chemical erosions; (9) surface segregation; and (10) graphical interface with built-in periodic table of elements and their properties. The ITMC-DYN code is based on the binary collision approximation (BCA) methods for modeling the transport and slowing down of incident ion beams in target materials and target atoms collision and mixing processes. For target evolution and modification, our model considers all target atoms generated cascades including implanted, sputtered, backscattered, diffused, and segregated atoms. However, the BCA is not valid at very low energies of <20 eV or so due to multiple atom interactions.

The collision models were integrated with detail models of time-dependent processes such as atom diffusion and segregation. Therefore, we considered actual fluxes and exact irradiation times of the experiments. The time step was determined from the processes of diffusion, molecular recombination, and surface segregation. An implicit method for modeling atoms diffusion was implemented to increase the time step and reduce the required computational time in the simulations especially for species with high diffusivity such as H in W. Additional surface boundary conditions were used to specify the recombination of a diatomic hydrogen isotope molecules and their release from the surface in modeling of both laboratory and reactor experiments [3].

Models developed for the chemical sputtering of carbon is based on the erosion yield that depends on target temperature, ions energy, and flux intensity [6]. The concentration and spatial profile of carbon atoms in mixed target materials and their surface segregation requires additional care in the evaluation of chemical erosion. Therefore, the total carbon erosion losses in our model are calculated in correspondence with the carbon concentration in each layer near the target surface.

Surface segregation was implemented based on the Darken model [7] that accounts for the segregation in binary alloys in terms of the difference in Gibbs free energy between surface and bulk [3]. The model for the surface segregation in the case of high surface enrichment factor is equivalent to the Fick's law of diffusion [7]. We used experimentally obtained coefficients and concentration dependent values without using any free parameters in our models.

3. Modeling results

To benchmark our models/code we considered the recent ITER-relevant experiments of plasma material interactions [4,8]. In these experiments, beams of hydrogen ions containing carbon impurity ions impinged on pure tungsten samples heated from 453 K to 1050 K. 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% of C ions with 1000 eV energy. Carbon concentration on the surface of tungsten was measured and conditions for blister formation were investigated with the dependence on the total fluence, on the percentage of carbon concentration in the ion beams, and on sample temperatures. We modeled the exact parameters of the above experiments and analyzed both the hydrogen accumulation inside the mixed target as well as carbon spatial concentration for the various target temperatures, ions fluences, and C impurity fraction used in the experiments.

3.1. Dependence of blisters formation on impurity concentrations

Three cases considered in the experiments regarding carbon impurity concentrations in ions beam were analyzed with respect to target modification and conditions of blister formation. Fig. 1 shows modeled and two experimental spatial distributions of C concentration in tungsten at temperature 653 K and H fluence of $3 \times 10^{22}$ H/cm² with 0.11%, 0.35%, 0.84% and 2% of C in ions beam. The lower content of carbon of 0.11% in comparison with 0.84% resulted in the following differences in samples: (1) the peak carbon concentration changed from 40% to more than 60%; (2) its location is shifted 15–20 nm from the surface in case of 0.11% and 7–8 nm in the case of 0.84%; and (3) target erosion is almost 10 times higher under the ion fluence containing 0.84% C. The difference in the target erosion explains the difference in the peak location. 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 beam. The shifted peak of carbon in the sample and its lower concentration reduced hydrogen retention and blister formation [8]. The models prediction showed the trend of the experimental data but not the actual spatial profile. The models results shown in this figure did not include post-irradiation surface segregation and etching.

![Fig. 1. Concentration of C in tungsten at temperature 653 K and fluence of $3 \times 10^{22}$ H/cm² with 0.11%, 0.35%, 0.84% and 2% of C in ion beam [4,8].](image-url)
3.2. Blister formation and the dependence on target temperature

Blister formation depends on the mobility of the implanted gas and on the concentration of gas atoms in the target. Accumulation of H in tungsten target in the considered experiments can be due to lattice imperfections, ion-induced damage (less importance for the low energies of incident H ions), and carbon atoms implantation. In these experiments carbon was deposited in the form of graphite or W2C on the sample surface. Fig. 2 shows comparison of the experimental data and modeling results of carbon concentration for different target temperatures, i.e., 453 K, 653 K, and 1000 K and for fluence of $3 \times 10^{20}$ H/cm$^2$ with carbon in the beam of 0.84%. Carbon diffusion was implemented in the model assuming a diffusion coefficient of C in W of $1 \times 10^{-15}$ cm$^2$/s at 1000 K; that is consistent with values obtained in more recent experiments and in modeling as well [9].

Diffusion of hydrogen in pure tungsten is high even for the lowest target temperature considered in the experiments and in modeling – with diffusion coefficient of $1 \times 10^{-23}$ cm$^2$/s for 453 K [10]. The rate of hydrogen molecular recombination at tungsten surface for these conditions is about $1 \times 10^{-25}$ cm$^3$/s [3,11]. Therefore, hydrogen deposited within a range of 5 nm can be easily recombined and released from the tungsten. The situation is, however, very different in composite materials containing W and C. For modeling of H diffusion in such composites we considered a combined “effective” diffusion coefficient as the interpolation of the logarithmic values of the individual diffusion coefficients of hydrogen in W and C according to their concentration. The diffusion coefficient of H atoms in randomly oriented carbon was taken from [12]. Carbon prevented the release of hydrogen from the surface and significantly increased H trapping in the bulk tungsten. It was reported in the experiments that high densities of blisters with sizes up to 20–30 μm were formed in the sample at a temperature of 453 K, large number of blisters were found in the sample at 653 K and no significant blisters were found in the case of samples irradiated at 1000 K [8].

3.3. Conditions for blisters formation and dependence on total fluence

Increasing the fluence in these experiments shown to enhance blisters formation. This is explained by the higher concentration of carbon in the sample at higher fluences and due to the thermal diffusion energy of hydrogen in tungsten at the temperature of 653 K that allows trapping of H atoms and accumulation in the bulk with time in areas with enriched carbon deposition. Fig. 3 shows dependence of carbon concentration in tungsten on the total fluence at sample temperature of 653 K and C concentration in the beam of 0.84%. The concentration of C in tungsten significantly increases with increasing the fluence from $3 \times 10^{18}$ H/cm$^2$ to $3 \times 10^{20}$ H/cm$^2$. The modeling results, which included effect of diffusion, surface segregation, chemical erosion, and etching are in good agreement with the data [3].

3.4. Effects of segregation and etching on carbon concentration in target

We implemented two additional and important processes to analyze the difference in the peak location of carbon concentration in the experiments and in our modeling, i.e., surface segregation and the effect of post-irradiation samples etching by Ar ions. The process of surface segregation moves carbon atoms from the bulk to the surface layer because of increasing the chemical potential of carbon in the bulk of W/C compound. This phenomenon will shift the peak of the carbon concentration profile closer to the surface. However, if we simulate this process self-consistently with the processes of ions beam deposition, target atoms sputtering, and atom cascade mixing, the effect of surface segregation alone loses its effectiveness particularly when we consider the appropriate values of the diffusion coefficient and the segregation energy at the given sample temperature. Fig. 4 demonstrates the effect of surface segregation on carbon profile as a function of different diffusion coefficients of carbon in tungsten at target temperature of 653 K and C concentration in the beam of 0.84%. Value of the segregation energy was found from the experiments given in Refs.
3.5. Steady-state erosion rate losses

To study the integrated effect of the various above modeled processes on the overall surface erosion we calculated the rates of mass losses of tungsten and the deposited carbon and hydrogen for the sample of temperature 653 K and the ions beam with 0.84% of C. Fig. 5 shows that surface erosion and dynamic target modification reach a steady-state condition after 1500 s of irradiation, which corresponds to a total fluence of 4.5 \times 10^{19} \text{H/cm}^2. The chemical erosion yield of carbon was calculated to be 1 \times 10^{-3} \text{atoms/ion}. This value takes into account sample temperature, ions energy and flux, hydrogen mass and carbon concentration in the target. After the steady state concentration reached, the deposited C atoms are sputtered at the same rate due to both physical and chemical sputtering of H and C ions in the incident beam.

4. Summary and conclusion

We upgraded our ITMC-DYN code that now includes the dynamic changing of material composition, deposition of simultaneous complex ions beams, atom diffusion, chemical erosion, surface segregation and recombination processes, and etching induced redistribution of target atoms. Modeling results and comparison with experiments showed good agreement and therefore, the advantage and potential use of computer simulation to predict and optimize the complex materials behavior in real fusion reactor environments.

The newly developed models successfully predicted the conditions for blister formation as shown in recent experiments. Parameters such as, the diffusion coefficient of hydrogen in carbon-rich zones can significantly influence the accumulation and the resulting profiles in candidate plasma facing materials such as tungsten. Self-consistent analyses of all processes involved in modeling material evolution during ions beam bombardment is quite important in the overall understanding of surface erosion, mixed materials evolution, and hydrogen isotope behavior and retention in plasma facing components. Low level of impurity contents in plasma, can significantly affect erosion lifetime, largely increase hydrogen isotope retention, and enhance bubble/blister formation in candidate reactor materials in fusion environments.

5. Concluded reference

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References
