Nuclear Materials and Energy 9 (2016) 571–575

Contents lists available at ScienceDirect

Nuclear Materials and Energy

journal homepage: www.elsevier.com/locate/nme

Atomistic simulations of deuterium irradiation on iron-based alloys in future fusion reactors

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ARTICLE INFO

Article history:
Received 13 November 2015
Revised 26 August 2016
Accepted 29 August 2016
Available online 14 October 2016

ABSTRACT

Iron-based alloys are now being considered as plasma-facing materials for the first wall of future fusion reactors. Therefore, the iron (Fe) and carbon (C) erosion will play a key role in predicting the life-time and viability of reactors with steel walls. In this work, the surface erosion and morphology changes due to deuterium (D) irradiation in pure Fe, Fe with 1% C impurity and the cementite, are studied using molecular dynamics (MD) simulations, varying surface temperature and impact energy. The sputtering yields for both Fe and C were found to increase with incoming energy. In iron carbide, C sputtering was preferential to Fe and the deuterium was mainly trapped as D_2 in bubbles, while mostly atomic D was present in Fe and Fe–1%C. The sputtering yields obtained from MD were compared to SDTrimSP yields. At lower impact energies, the sputtering mechanism was of both physical and chemical origin, while at higher energies (>100 eV) the physical sputtering dominated.

1. Introduction

One of the major challenges for future fusion reactors is the development of materials that will withstand the intense flow of a high energy plasma, due to non-perfect plasma confinement [1]. Various steels are being considered as plasma-facing materials (PFMs) for the main wall of DEMO, the main power-plant scale fusion reactor project [2]. The interest to this possibility was raised in particular by the recent realization that steels that have been made to have reduced activation by adding W, can have strongly reduced erosion due to preferential sputtering causing W enrichment at the surface [3]. However, for a steel to be viable as a PFM, certain qualities must be met, the most crucial issue is the lifetime of the steel, strongly affected by different erosion mechanisms. Since steels are alloys of iron (Fe) and carbon (C) (for instance, in the EUROFER steels planned to be used in DEMO, the carbon content is about 0.5 atomic % [4]), it is of vital importance to quantify the erosion of both elements when being exposed to hydrogen plasma, such as deuterium (D). Moreover, since steels in general have a complex microstructure and may contain, in addition to the basic iron phases, like austenite and ferrite, also carbide in layer and particles [5], it is also important to understand the sputtering of iron carbides.

Several experiments have been carried out to study sputtering of pure iron and that of steel containing some carbon over a wide range of irradiation energies [6,7]. However, little attention has been drawn to plasma-surface interactions (PSIs) of steel targets exposed to D plasma, and the preferential sputtering and depletion of C. In order to gain insight into the atomic processes and to make an assessment about the possible role of steel as PFM candidate, atomistic simulations are required.

In this work, we used molecular dynamics (MD) simulations to analyze the effect of D irradiation on ferrite, pure body-centered cubic (BCC) Fe, Fe with 1% C impurity (Fe–1%C) and the iron carbide (Fe_3C), under different irradiation energies and substrate temperatures. Since chemical effects during ion irradiations can be studied with MD, we compared our results to sputtering yields calculated with the dynamic binary collision approximation (BCA) code SDTrimSP [8]. Special attention was paid to sputtering behavior of C in Fe_3C.

2. Method

2.1. Molecular dynamics simulations

Molecular dynamics (MD) simulations is a computational method capable of describing bond formation and breaking when

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http://dx.doi.org/10.1016/j.nme.2016.08.021

Table 1
Set-up characteristics of the molecular dynamics simulations, for pure iron (Fe), 1%-carbon (C) containing Fe and iron carbide (Fe_3C). The table specifies the number of atoms in the initial MD structure (N), the size of the initial structure, the surface temperature (T), the ion impact energy (E) and flux.

Structure	Fe	Fe–1%C	Fe_3C
N	3200	3232	2000
Size (nm)	$2.9 \times 2.9 \times 4.6$	$2.9 \times 2.9 \times 4.6$	$2.5 \times 3.8 \times 2.3$
T (K)	300, 400, 500, 600, 800	500	500
E (eV)	30, 40, 50, 70, 100, 200, 500	20, 40, 50, 70, 100, 150, 200	20, 40, 50, 70, 100, 150, 200
Flux (10^{28} m^{-2} s^{-1})	1.2	1.2	1.36

suitable reactive interatomic potentials are used. Consequently, it is an excellent tool for studying the erosion of chemically active structures. The code PARCAS [9] was used for MD simulations presented in this work. An analytical bond-order potential [10] was used to calculate interatomic forces in the binary Fe-D systems. To model the ternary Fe–C–D systems, the potential calculation was modified in such a way that C–C, C–D and D–D parameters are given by Brenner's second parametrization [11], while for bonds involving Fe atoms, the Fe–C potential [12] was used. Moreover, the formalism of Fe-C-D potential is based on formulation by Tersoff [13] and Brenner, and it has been shown to be suitable for describing both metallic and covalent bonds [14].

The MD simulations were carried out in two main steps: first the initial structure for pure Fe, Fe–1%C and Fe_3C was prepared, after which the cell was irradiated with 5000 cumulative D irradiations for pure (110) BCC Fe and Fe–1%C, and 3000 cumulative D irradiations for Fe_3C at normal incidence angle.

The initial simulation cells were created by relaxing the structures at the desired temperature, and opening a perfectly flat surface normal to the z-direction. In the Fe–1%C, the C atoms were inserted in randomly selected octahedral sites. After the relaxation, these surfaces were irradiated with cumulative D impacts varying the impact energy and substrate temperature. Each D impact simulation lasted for 7 ps.

Further details regarding to methodology, such as temperature and pressure control, use of electronic stopping and periodic boundary conditions can be found in Ref. [15]. The characteristics of each simulation cell and D ion parameters are listed in Table 1.

2.2. SDTrimSP

SDTrimSP is a BCA code suitable for simulation of atomic collisions in structure-less targets. In this work, SDTrimSP simulations were performed to provide comparison to the MD results. Fe_3C substrate was subjected to D ions with 50, 100, 150 and 200 eV energy. The fluence in all simulations was set to be 5×10^{16} m^{-2} .

It should be noted that in SDTrimSP no chemical effects are taken into account, therefore, the BCA approximation becomes unreliable at impact energies lower than 50 eV for heavy materials [16] like Fe and C. However, the code is reliable at high energies, and comparing the results with MD, where chemical effects have been taken into account, can provide important information about the underlying mechanisms.

3. Results and discussion

3.1. Pure Fe and Fe–1%C surfaces

Fig. 1 shows the total Fe sputtering yield as a function of surface temperature and D impact energy. Over all, the sputtering yield increases with the impact energy above 100 eV, the yields rapidly increase, as more kinetic energy is available for bond breaking. At impact energies above 200 eV, the yields begin to saturate.

The sputtering yields shown in Fig. 1 have no significant temperature (T) dependence within the range studied here. Therefore,

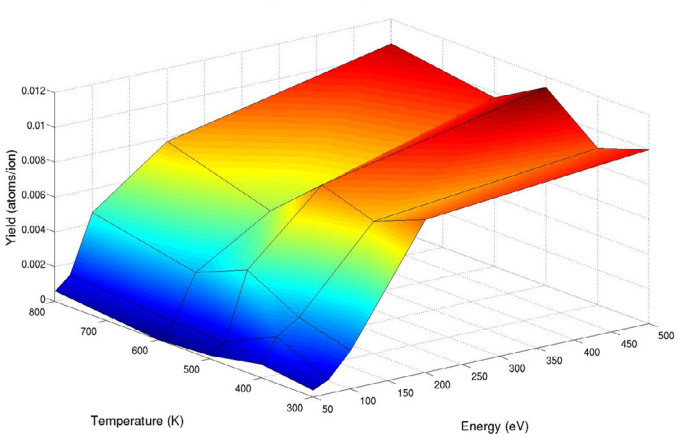

Fig. 1. Total Fe sputtering yield as a function of surface temperature and impact energy after 5000 cumulative D impacts for pure Fe.

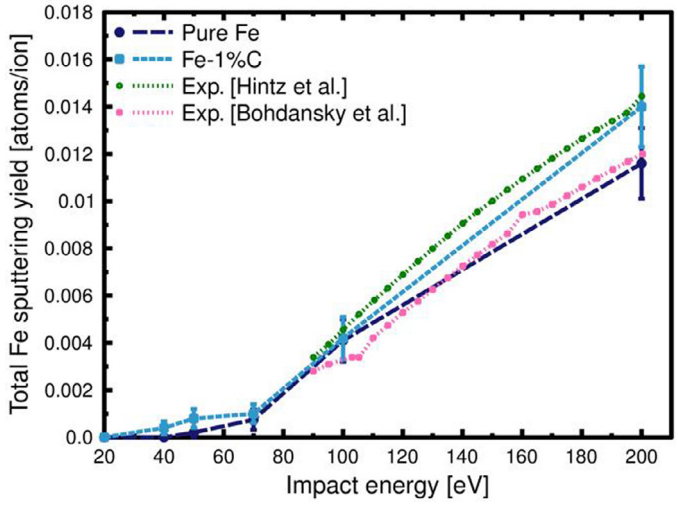

Fig. 2. A comparison of Fe sputtering yields in pure Fe and Fe–1%C between MD simulations and experimental data at different impact energies. In the simulations, the temperature was set to 500 K.

and due to limitations in available computational resources, the rest of simulations were carried out at T = 500 K, with varying D impact energy. Fe molecular sputtering was found to be negligible in these simulations.

In Fig. 2, Fe sputtering yields for pure Fe, and for Fe–1%C are compared to the experimental outcome by Hintz et al. [7] and by Bohdansky et al. [6], for D impact energies between 90 and 200 eV The results show excellent agreement between simulations and experiments.

Fig. 3 shows the fraction of D atoms not implanted in the pure Fe, and the Fe–1%C, simulations cells. Those atoms were either reflected from the surface or released as molecules. The figure shows