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Aging simulations of plasma facing materials through a multiscale approach

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ABSTRACT

Understanding the fusion reactors physics is critical to designing the energy supply of the near future. One of the efforts to reach, concerns the damaging evolution description of plasma facing materials (PFMs).
In this environment, predictive tools, based on multiscale approaches, are necessary to estimate properly the phenomena leading to the PFM microstructural modifications.
During NuMat 2022, we presented the first result of an open-source erosion simulator based on multiscale modeling. Although the tool is still in the calibration stage, it seems able to predict the nanoscopic evolution of PFMs showing a non-trivial dependence from the initial parameters.
The computational model is based on the sequential combination of a plasma global code (surface geometry provided) and a feature scale particle-like Kinetic Monte Carlo (KMC) tool.
The global model allows the thermodynamic and stoichiometric description of plasma state together with the related sheath potential evaluation.
The three-dimensional KMC simulates the sequences of surface and near-surface structural modifications caused by plasma particles impinging a facing slab. Subsequently, particles can migrate or bind the lattice of the PFM.
In this presentation, we will show the content of our adapted NuMat 22 talk, with useful technical information for those interested in using the code.

Video and Presentations to this article can be found online at https://doi.org/10.1016/j.sctalk.2023.100182.

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Figures and tables

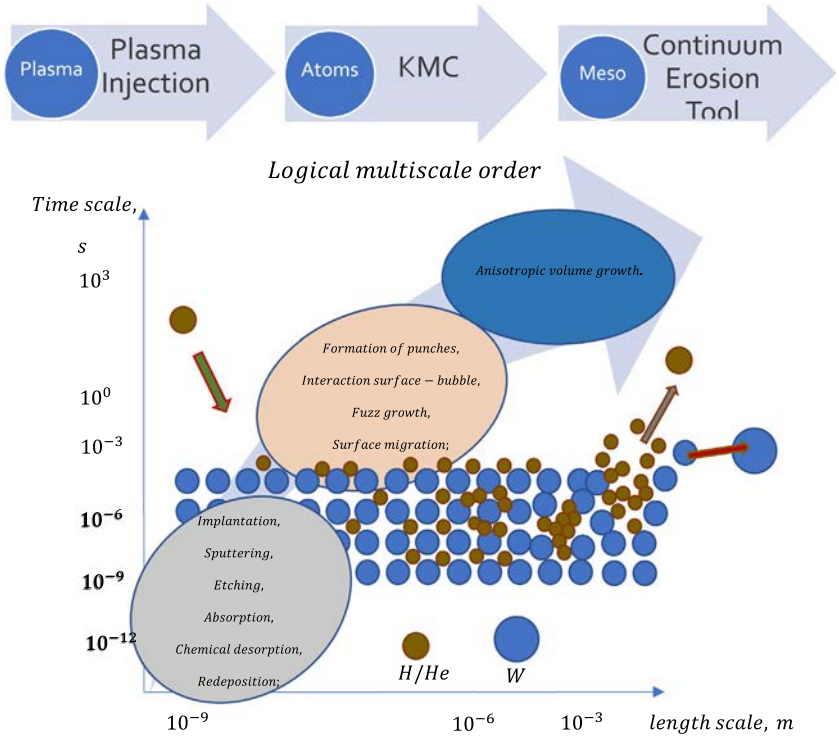

Fig. 1. Multiscale structural evolution of materials in nuclear fusion. Many processes at numerous time and spatial scales occur on a reactor wall, including: Implantation, Sputtering, Etching, Interaction surface-bubble, Fuzz growth, etc. See the review of Marian et al. [1] for a more detailed description of all the possible involved processes.

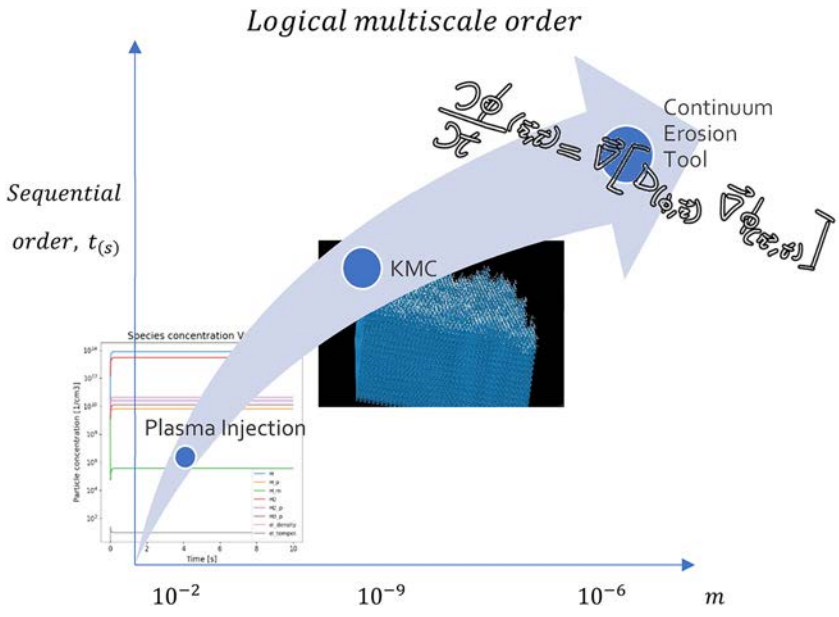

Fig. 2. Multiscale structural evolution: materials and tools. To concretely solve the problem of physical processes acting on multiple scales, we decided to follow the physics with our codes by dividing our approach into three main tools that communicate with each other. The first two are presented.

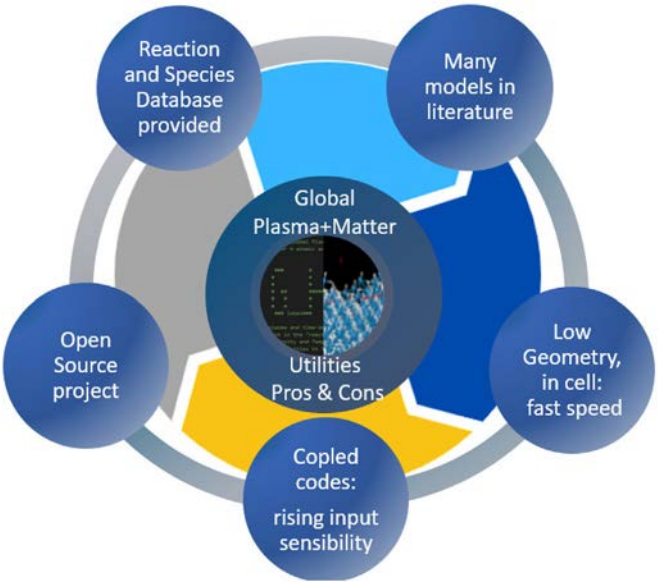

Fig. 3. Pros and cons of our multiscale approach. Our approach is based on two coupled codes, so we describe the advantages and disadvantages of this model. Both tools need supporting databases in terms of reactions and species. We programmed our codes to make some geometrical approximations resulting in a great advantage in execution speed. Coupling two codes means increasing the sensitivity of the overall system.

```
#******************************************************  GlobalPlasma_H  ****************************************
#                                  Version 1.1                    date: 23/06/2022
#                                          Global Plasma 0D Simulator
#                                       for H atomic and molecular plasmas
#
#
#                                     ###        #    #
#                                    #           #    #
#                                    #           #    #
#                                    #  ##       ######
#                                    #   #       #    #
#                                    #   #       #    #
#                                     ### lobal###    ## 0D Plasmas
#
# This code simulates the steady state of plasma and time-dependent solutions for atomic and molecular gases.
# Geometry and kinetics are taken into account in the "reaction parameters"
# Prints two png files: - outelec (Electron Density and Temperature Vs Time [s])
#                       - outDensity (Species Densities Vs Time [s])
# Authors:                          A. La Magna                    G. Lo Presti
# CNR IMM Catania

import matplotlib.pyplot as plt
import sys
import os
from math import *
import numpy as np
from scipy.optimize import root
from scipy.integrate import solve_ivp
```

Fig. 4. Global Plasma Code, figurative image representing the source of our code.

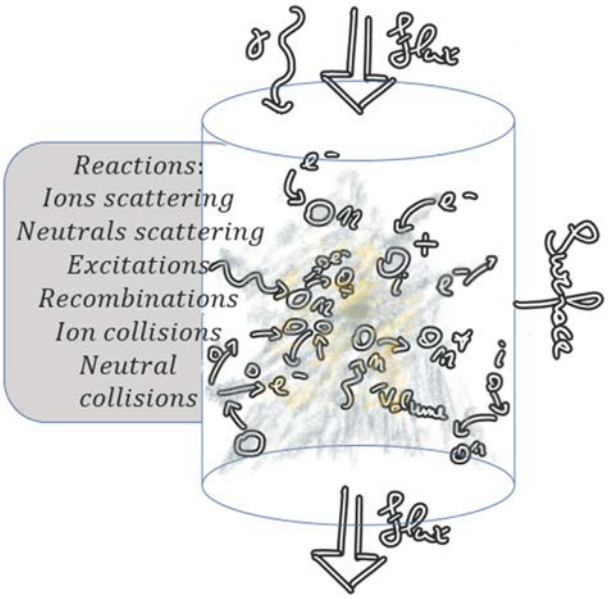

Fig. 5. Reactions example. When the gas enters the reactor, and energy is supplied to activate the plasma, our code predicts the surface area and volume reactions provided by databases. It is possible to include many types of processes among the reagents, for example: scattering, excitations, ionizations, recombinations, collisions and so on.

```
<Reactions xmlns="http://www.imm.cnr.it/ETCH/Reaction">
    <Reaction >
      <Name Value="R35" />
      <Coefficient Name="KR35" Value="Ti_eV/(8.61800806184e-5*298.15)" />
      <Threshold Name="ER35"   Value="0" /><!-- Antonio Zecca; Grzegorz P. Karwasz; Roberto S. Brusa (1996).-->
      <Loss>
          <Specie Name='H2' />
        </Loss>
      <Product>
          <Specie Name='H' />
          <Specie Name='H' />
      </Product>
    </Reaction>
```

Fig. 6. Inserting Reactions: a demonstrative example of reaction in our database. To enter a new reaction, just indicate the name of the reaction and the reaction parameters: particles, rate, and threshold.

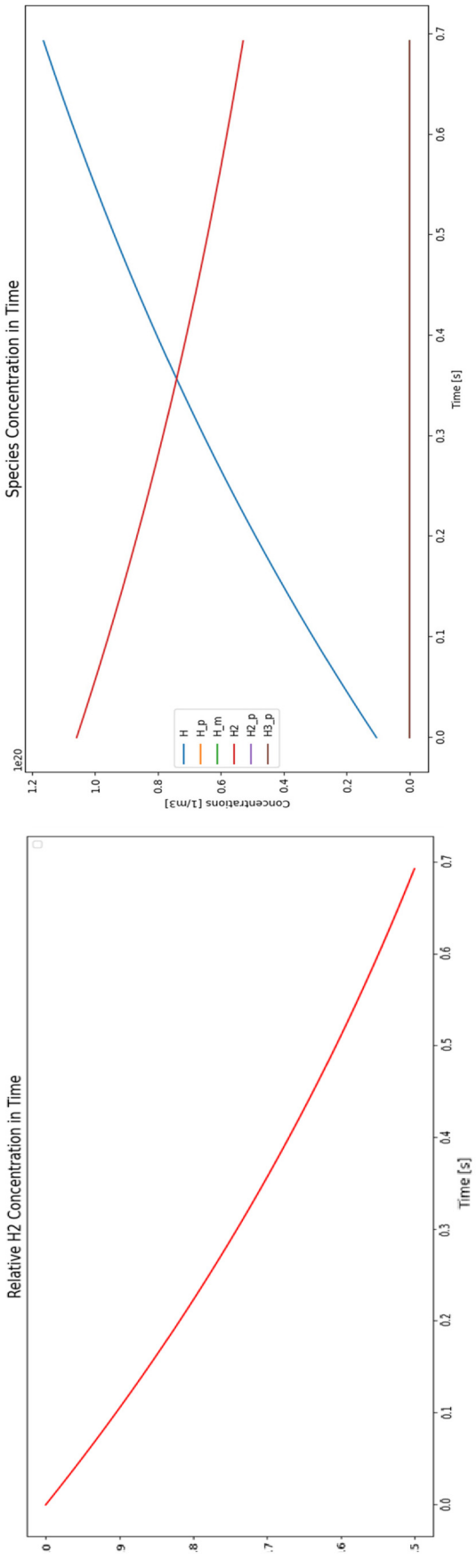

Fig. 7. Demo H2 Reaction: concentration Vs Time. This image represents the result of a demonstrative reaction in which molecular hydrogen breaks down into two atomic hydrogen particles. The rate has been set equal to 1, so in 0.7 s the code halves the initial amount of hydrogen. The other species are not involved in the reaction and remain constant.

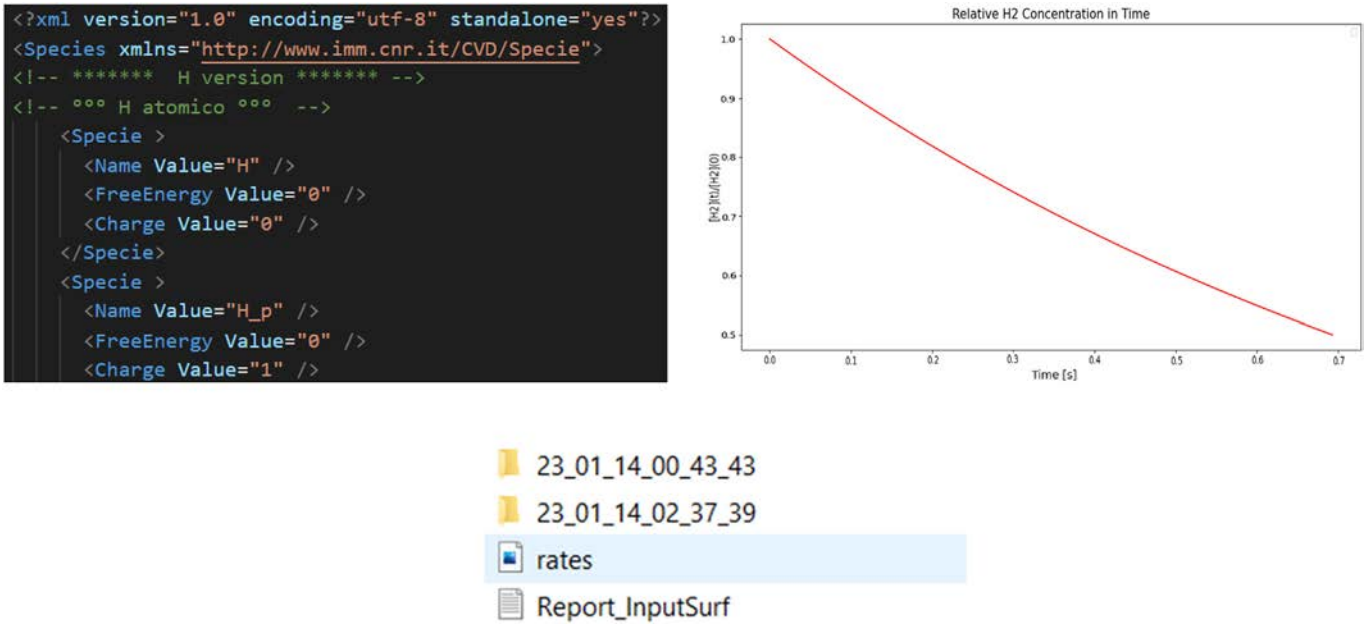

Fig. 8. logical code structure. This image illustrates some details of the logical structure of the folders in our plasma code. In the main folder there are three subfolders: Database_preprocessing, Main, and Results. The parameters that users are interested in (power, pressure, number of iterations, etc.) are in the main code.

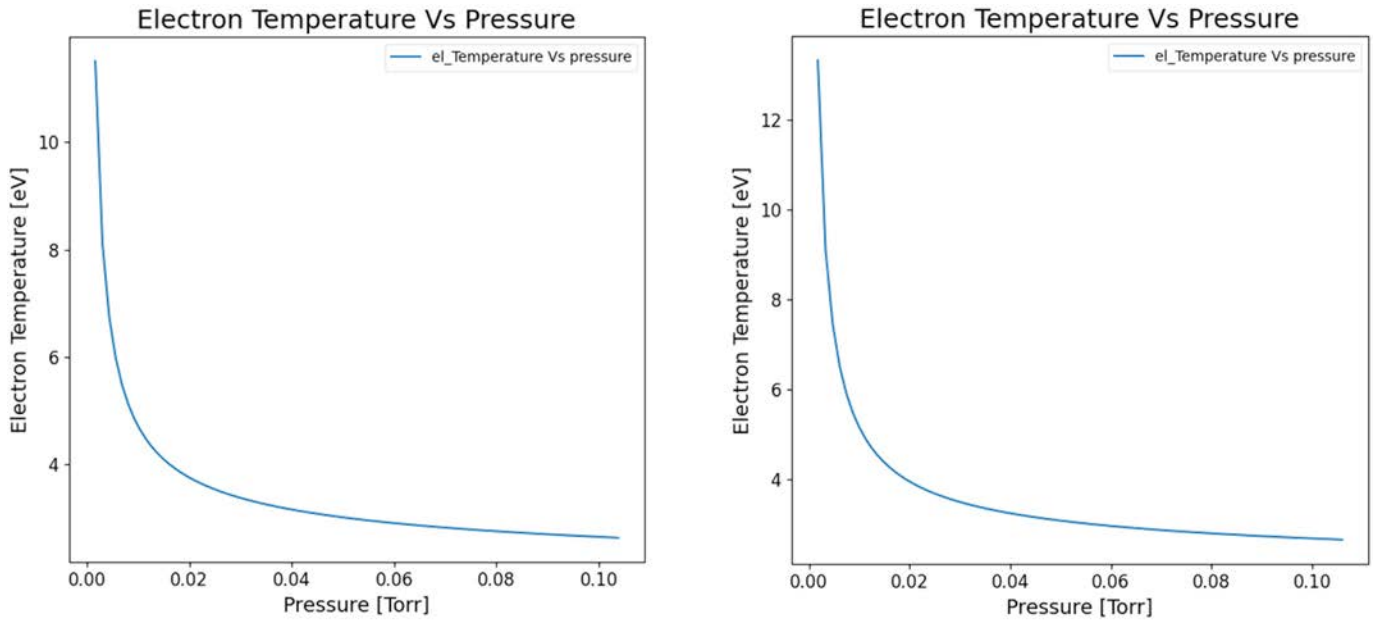

Fig. 9. Demonstrative plot of Electron Temperature Vs Pressure. Cylinder of L = 40 cm, R = 10 cm; Tgas = 500 K. On the left side the case for 800 W, at the right side the one for 1200 W.

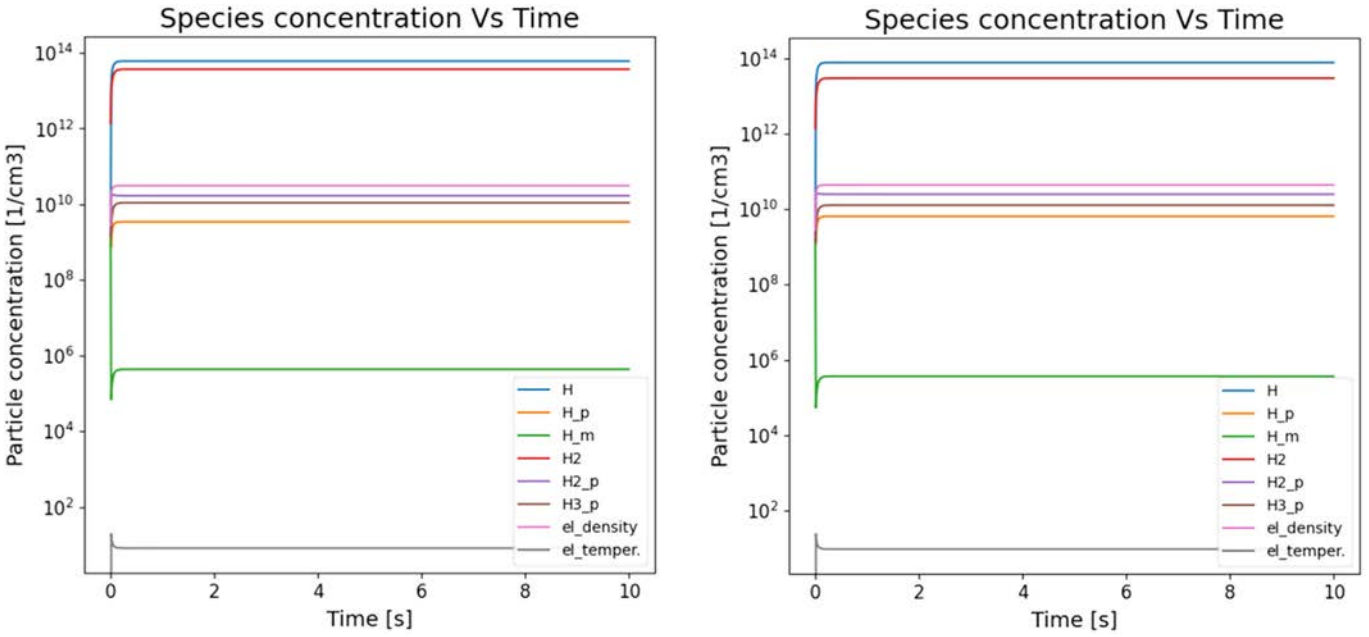

Fig. 10. Demonstrative plot of Concentration Vs Time. Cylinder of L = 40 cm, R = 10 cm; Tgas = 500 K, Pressure = 1mTorr (H_2). On the left side the case for 800 W, at the right side the one for 1200 W.

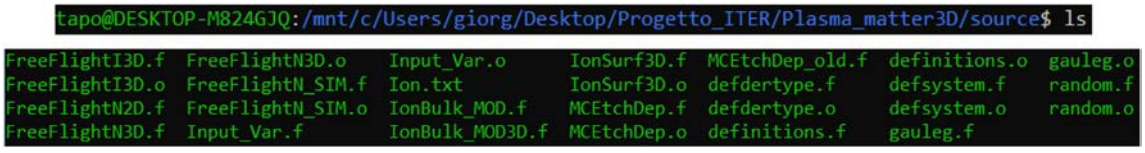

Fig. 11. How our code looks inside: this is the file structure of our source file. Image referred to table 2: Combination compounds for Surface MC Reactions [3]. A cell number must be assigned in each cell according to each type of particle. For each reaction, for each species, the MC calibration must be chosen and inserted like in Table 2. This is a piece of our surface sticking routine for H plasma on W surface bcc.

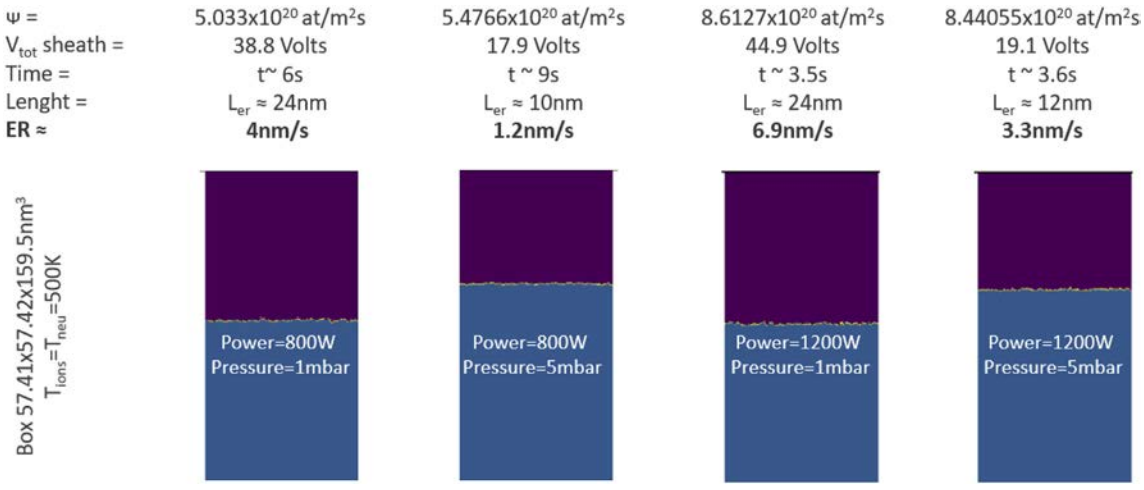

Fig. 12. kMC dependences. It represents various simulations varying power and pressure on a W unit cell a_W = 0.319 nm as KMC lattice unit - Fixed dose comparisons: Total Dose 3.033×10^{21} at/m^2. The contextual change of the parameters does not lead the system to respond in a trivial way. Although more in-depth analysis is needed, the erosion length seems to depend mainly on the sheath potential. Longer erosion lengths correspond at lower pressures, and there is a weak dependence on power. The erosion speed increases with the power.

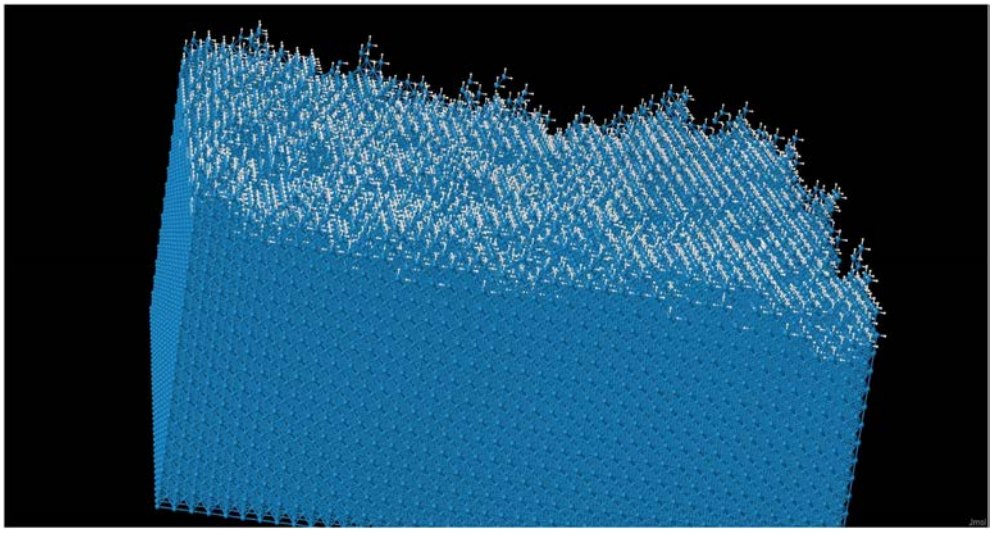

Fig. 13. MC erosion atomic detail. This image is from one of the first simulations with our Monte Carlo code. The 3D imaging of our code reaches the quasi-atomic sensitivity.

Table 1
Coefficients of Plasma Volume and Surface Reactions [2,4].
To guarantee a correct plasma simulation, a closed set of reactions must be inserted, divided into volume and surface reactions (those indexed from 100 onwards). A threshold and a rate must then be coupled to each reaction.

Name	Reaction
R1	$H_2 + e^- \rightarrow H_2^+ + e^- + e^-$
R2	$H_2 + e^- \rightarrow H + H + e^-$
R3	$H_2 + e^- \rightarrow H + H^-$
R4	$H + e^- \rightarrow H^+ + e^- + e^-$
R5	$H + H_2^+ \rightarrow H_2 + H^+$
R6	$H_2^+ + e^- \rightarrow H + H^+ + e^-$
R7	$H_3^+ + e^- \rightarrow H_2^+ + H^-$
R8	$H_2 + H_2^+ \rightarrow H + H_3^+$
R9	$H^+ + H^- \rightarrow H + H$
R10	$H_2^+ + H^- \rightarrow H + H + H$
R11	$H_3^+ + H^- \rightarrow H + H + H + H$
R12	$H^- + e^- \rightarrow H + e^- + e^-$
R13	$e^- + H_3^+ \rightarrow H + H + H^+ + e^-$
R14	$H_2^+ + e^- \rightarrow H + H$
R15	$H_2 + H^+ \rightarrow H_3^+$
R16	$H_3^+ + e^- \rightarrow H + H + H$
R17	$H_3^+ + e^- \rightarrow H + H_2$
R101	$H + wall \rightarrow H_2$
R101a	$H + wall \rightarrow$
R102	$H_2 + wall \rightarrow H_2$
R103	$H^+ + wall \rightarrow H$
R104	$H_2^+ + wall \rightarrow H_2$
R105	$H_3^+ + wall \rightarrow H + H_2$

Name	Reaction	Cofficient $\left[{}^{cm^3}/_{s}\right]$	Threshold [eV]
R34	$H_2 + e^- \rightarrow H_2^+ + e^- + e^-$	$1.10^{*}10^{-14} T_e^{0.42} e^{-16.05/T_e}$	15.43

CRediT authorship contribution statement

Giorgio Lo Presti: Investigation, Data curation, Writing – original draft, Software. **Antonino La Magna:** Methodology, Supervision, Software.

Data availability

No data was used for the research described in the article.

Acknowledgments

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Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Further reading

[1] Hydrogen Plasmas and Their Interaction with Fusion-Relevant Materials, Cameron Mclnnes Saimuell, A thesis of Doctor of Philosophy for Australian National Universit, July 2014.
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Antonino La Magna received his master's in physics (cum laude) and his Ph.D. in Physics at the University of Catania in 1992 and 1996, respectively. Since 1999, he has been a permanent staff member (from 2010 as Senior Researcher, from 2020 as Director of Research) at the Institute for the Microelectronics and Microsystems of the Italian National Council of Research (CNR-IMM), where he is responsible of the computational team (1999-Today). Currently, he leads the research group on advanced processes (2010-Today) and he is coordinator and responsible for the CNR-IMM of several international projects on behalf of industry. He has authored over 350 publications in international journals in the fields of solid-state physics, technological processes, and device simulations, and he is a frequently invited speaker at international conferences.

Giorgio Lo Presti is an Italian PhD student in theoretical physics. Immediately after his bachelor's degree, he attended the Interuniversity School of Mathematics and subsequently started a collaboration with the Cosmology and Fundamental Interactions group of the University of Basel to work on special issues in General Relativity (GR), producing his thesis “A study on Oscillons in Full GR”. To complete his studies, in came back in Catania where first he graduated in Theoretical Physics and then began his doctoral studies. Currently affiliated to the CNR-IMM, his main interests concern the evolution of surfaces passing from mathematical aspects of differential geometry to nuclear plasma physics. He is also a collaborator of the JRA Eni project which aims to produce green energy from nuclear fusion.