

# Multi-Scale Modelling to Relate Beryllium Surface Temperature, Deuterium Concentration and Erosion in Fusion Reactor Environment

E. Safi<sup>a</sup>, G. Valles<sup>b</sup>, A. Lasa<sup>c</sup>, K. Nordlund<sup>a</sup>

<sup>a</sup>*University of Helsinki, PO Box 43, 00014 University of Helsinki, Finland*

<sup>b</sup>*Instituto de Fusión Nuclear, Universidad Politécnica de Madrid, Madrid, Spain*

<sup>c</sup>*Oak Ridge National Laboratory, Oak Ridge, TN 37920 USA*

Beryllium (Be) has been chosen as plasma facing material for the main wall of ITER, the next generation fusion reactor. Identifying the key parameters that determine Be erosion under reactor relevant conditions is vital to predict the ITER plasma facing component lifetime and viability. To date, a certain prediction of Be erosion, focusing on the effect of two of such parameters, surface temperature and D surface content, has not been achieved. In this work, we develop the first multi-scale KMC-MD modeling approach for Be to provide a more accurate database for its erosion, as well as investigating parameters that affect erosion. First, we calculate the complex relationship between surface temperature and D concentration precisely by simulating the time evolution of the system using an object kinetic monte carlo (OKMC) technique [1]. These simulations provide D surface concentration profile for any surface temperature and incoming D energy. We then describe how this profile can be implemented as a starting configuration in molecular dynamics (MD) simulations. We finally use MD simulations to investigate the effect of temperature (300-800K) and impact energy (10-200eV) on the erosion of Be due to D plasma irradiations. The results reveals a strong dependency of the D surface content on temperature. Increasing the surface temperature leads to a lower D concentration at the surface, because of the tendency of D atoms to avoid being accommodated in a vacancy, and de-trapping from impurity sites and diffuse fast toward bulk. At the next step, total and molecular Be erosion yields due to D irradiations are analysed using MD simulations. The results show a strong dependency of erosion yields on surface temperature and incoming ion energy. The total Be erosion yield increases with temperature for impact energies up to 100 eV. However, increasing temperature and impact energy results in a lower fraction of Be atoms being sputtered as BeD molecules due to the lower D surface concentrations at higher temperatures. These findings correlate well with different experiments performed at JET and PISCES-B devices [2-3].

[1] I. Martin-Bragado, A. Rivera, G. Valles, J. Gomez-Selles, M. Caturla. *Comput. Phys. Commun.* 184 (2013) 2703–2710.

[2] S. Brezinsek, M.F. Stamp, D. Nishijima, D. Borodin, S. Devaux, K. Krieger, S. Marsen, M. O'Mullane, C. Bjoerkas, A. Kirschner and JET EFDA contributors. *NF.* 54 (2014) 103001

[3] D. Nishijima, R. P. Doerner, M. J. Baldwin, G. Temmerman. *J. Nucl. Mater.* (2009) 390–391

\*Corresponding author: tel.: +35 8451 680346, e-mail: [elnaz.safi@helsinki.fi](mailto:elnaz.safi@helsinki.fi) (E. safi)