The Projectile Effect in Sputtering of Ice and Liquid Water – Molecular Dynamics Simulations

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Secondary Ion Mass Spectrometry (SIMS) is a robust technique for 3D imaging of inorganic, organic, and biological systems, which offers unparalleled sensitivity and spatial resolution. Recently, Yang et al. extended this method to the analysis of samples in a liquid environment [1]. It was achieved using a microfluidic channel whose upper side was drilled by an ion beam to create a 2-3 µm window. The successive bombardment induced the emission of molecules from the exposed fluid, allowing for studying, among others, photochemical reactions, biofilms, and liquid-liquid interfaces [2].

Our knowledge of the mechanisms involved in the sputtering of liquids is currently limited. Information depth, molecule fragmentation rate, number of ejected molecules (sputtering yield), and the effect of temperature on the sputtering mechanisms are just a few examples of unknowns. We used reactive molecular dynamics (MD) simulations to gain insight into these phenomena by modelling the impacts of bismuth (Bi_n) and argon (Ar_n) clusters into water and ice samples. Our results show that the system behavior depends on the projectile used (Fig. 1) and the initial temperature of the sample.

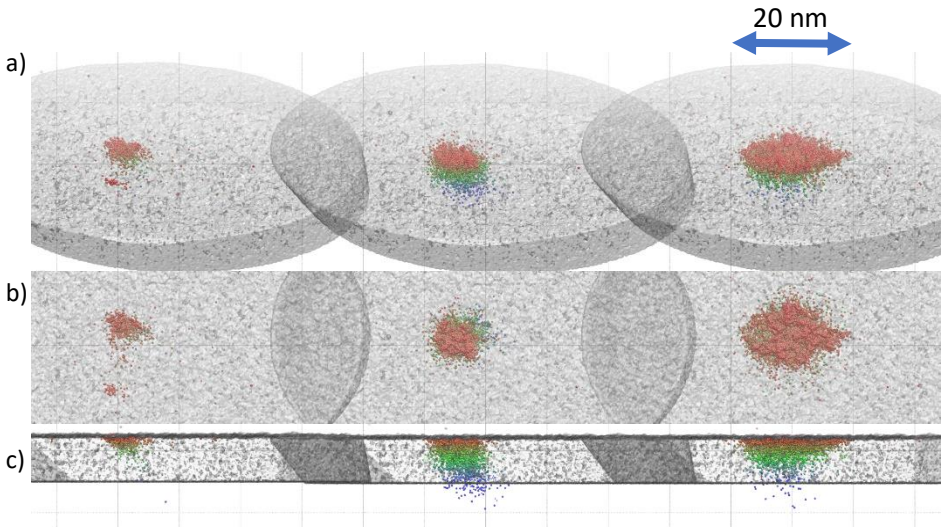

Fig. 1. a) Oblique, b) top, and c) side view of initial positions of sputtered water molecules during bombardment by Bi, Bi_3, and Ar_{1000} projectiles. The color scale corresponds to the initial depth of the ejected atoms. Lower parts of the systems are omitted, and images partly overlap for increased visibility.

This work was supported by a Polish National Science Centre Grant 2019/33/B/ST4/01778. MD simulations were performed using the PLGrid infrastructure.

[1] Yang, Li. *et al.,* Lab on a Chip, 11, 2481(2011)
[2] Yu, Xiao-Ying, Journal of Vacuum Science & Technology A, **38**, 040804(2020)