SUPPLEMENTARY MATERIAL for

***In situ atomic force microscopy depth-corrected 3-dimensional focused ion beam based time-of-flight secondary ion mass spectroscopy: spatial resolution, surface roughness, oxidation***

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Supplementary Table 1: Data of the sputtering progress.

|  |  |  |  |
| --- | --- | --- | --- |
| Frame number | Roughness  [nm] | Crater depth  [nm] | Sputter depth/20 frames  [nm] |
| 1 | 104.4 | 0 | 0 |
| 2 | 71.9 | 40.2 | 40.2 |
| 3 | 47.5 | 87.5 | 47.3 |
| 4 | 29.2 | 154.2 | 66.7 |
| 5 | 34.6 | 198.7 | 44.5 |
| 6 | 20.7 | 265.0 | 66.3 |
| 7 | 17.6 | 321.7 | 56.7 |
| 8 | 17.2 | 368.3 | 46.6 |
| 9 | 9.9 | 435.4 | 67.1 |
| 10 | 15.5 | 485 | 49.6 |
| 11 | 8.0 | 535 | 50 |
| 12 | 7.1 | 590 | 55 |
| 13 | 6.2 | 630 | 40 |
| 14 | 6.6 | 683 | 53 |
| 15 | 5.6 | 737 | 54 |
| 16 | 4.9 | 787 | 50 |
| 17 | 5.2 | 837 | 50 |
| 18 | 4.8 | 883 | 46 |
| 19 | 5.0 | 929 | 46 |
| 20 | 6.9 | 954 | 25 |
| 21 | 9.0 | 987 | 33 |
| 22 | 7.2 | 1006 | 19 |
| 23 | 6.4 | 1019 | 13 |
| 24 | 5.5 | 1037 | 18 |
| 25 | 7.3 | 1075 | 38 |
| 26 | 9.5 | 1106 | 31 |

Supplementary example: the creation of 20 nm slices for the 3D reconstruction:

Assuming that the first two sets of (containing 20 subsequent) ToF-SIMS frames correspond to 40.2 nm depth measured by AFM (Frame No. 2 in Suppl. Table 1), then in order to create segments that contain ToF-SIMS data from 20 nm (±1.5 nm) thick slices, (as 40.2 nm/ 20 frames = 2.01 nm for one frame in this set) the first slice contained the integrated values of the first 10 frames (corresponding to 20.1 nm thickness), while the second slice contained the integrated values of the frames 11-20 (with the same 20.1 nm thickness). Calculating the average depth for each sets of frames based on the AFM measurements the same way, the sufficient number of frames were integrated to have the same 20 nm thickness.