

Towards Accurate Atom Scale Characterisation of Hydrogen Passivation of Interfaces in TOPCon Architectures

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Supporting Information

Supporting data is included here showing:

1. The complete mass spectrum of the TOPCon specimen obtained in the APT experiment including a label of all peaks and potential overlaps. Figure S1.
2. An example of the use of AtomProbeLab (v.0.2.4) to obtain solved peaks in the overlap group 28-32 Da, produced using. Figure S2.
3. A zoom in to an atom map for the 16 Da and 31 Da species, indicating that the APT reconstruction algorithm produces a non-flat tunnelling oxide interface. Figure S3.
4. SIMS depths profiles of species in at/cm^3 for an equivalent TOPCon sample, recorded by CAMECA IMS 4fE6, and its comparison to APT data. Figure S4.
5. Concentration profiles along depth for ionic species of interest without overlap solving. Figures S5 and S6.

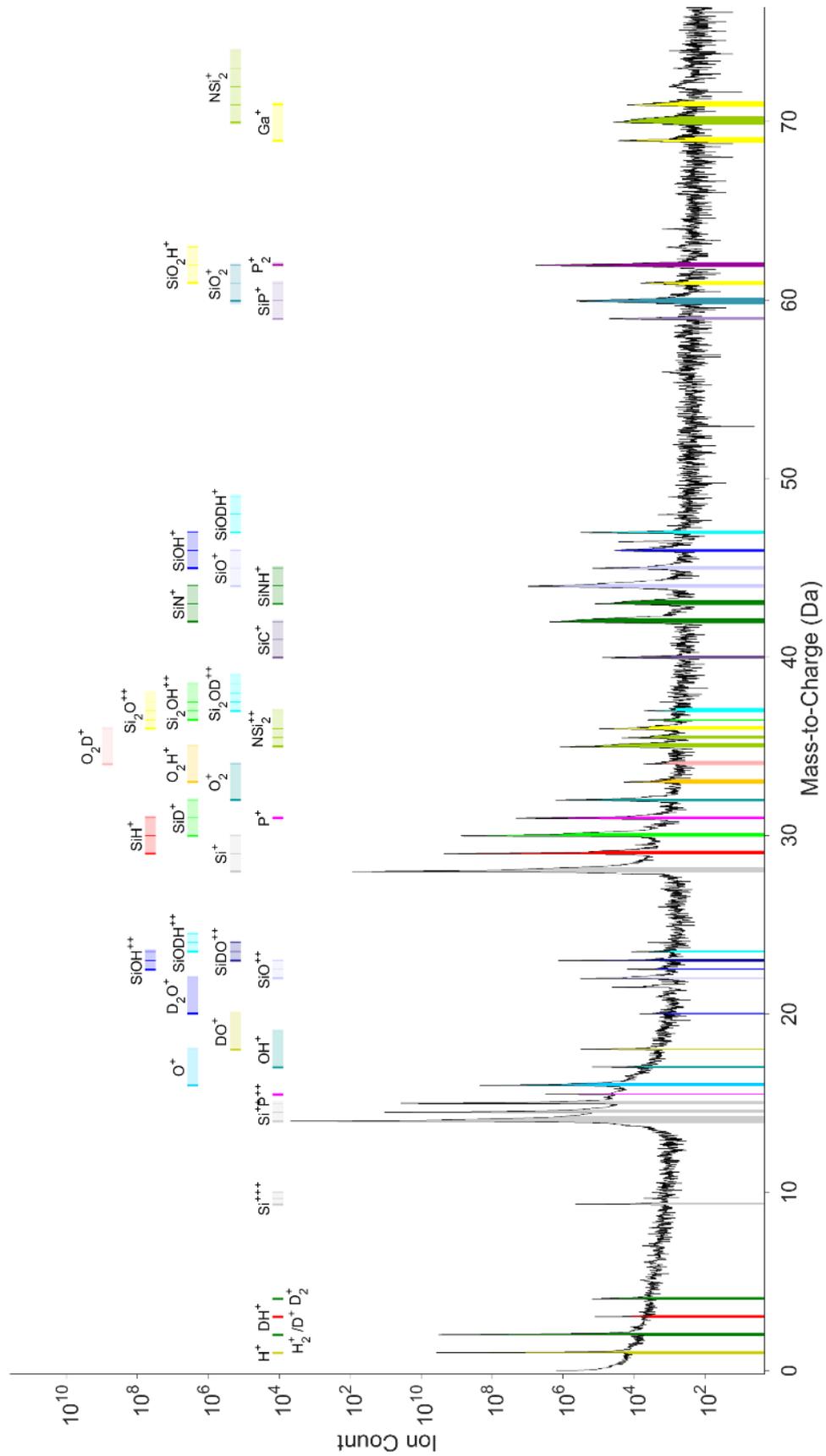


Figure S1. The mass spectrum of a complete TOPCon specimen obtained from the APT experiment, with peaks are ranged and labelled. The identified species present overlaps as they stack on top of certain peaks.

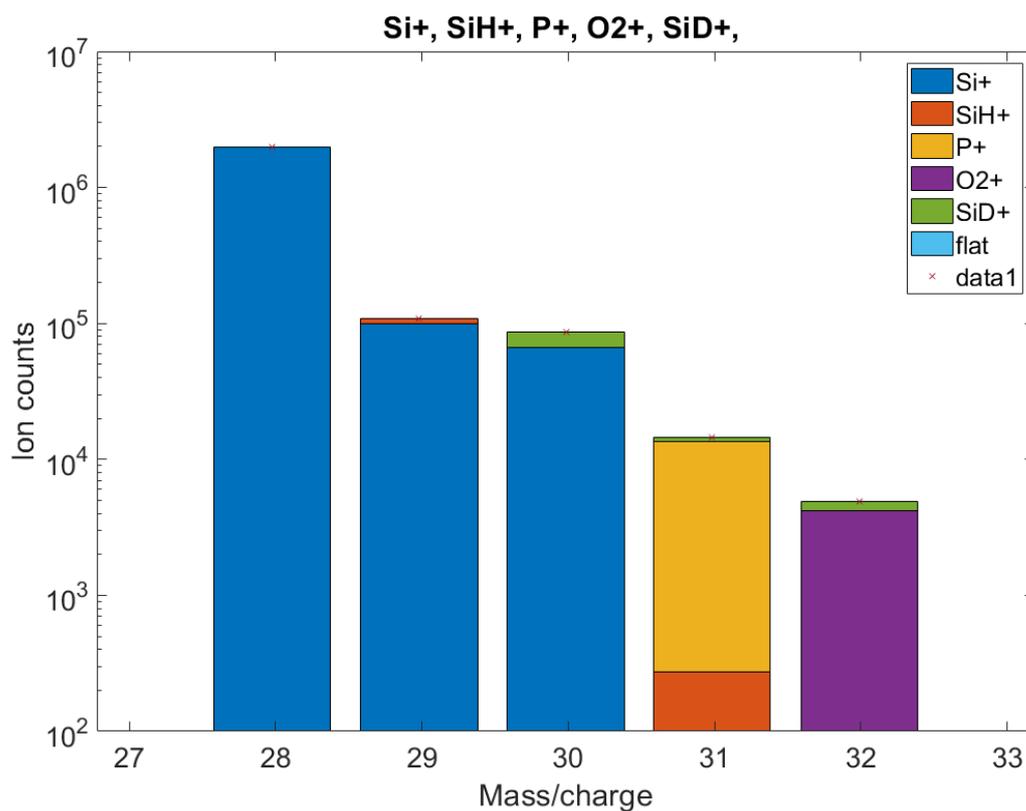


Figure S2. Example histogram of solved peaks within the overlap group 28-32 Da, produced using AtomProbeLab (v.0.2.4). The coloured bars give the fitted contribution of each ionic species to each peak. The cross marks the peak counts as obtained from the APT mass spectrum.

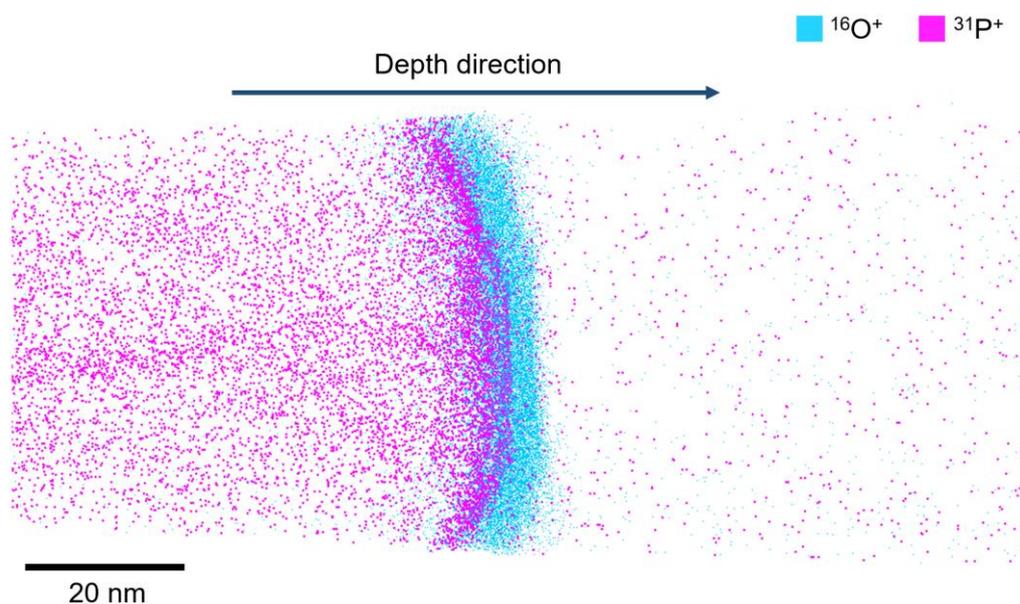


Figure S3. Magnified atom map for the 16 Da and 31 Da showing the non-flat oxide layer from APT reconstruction. This leads to spread-out of composition profiles when plotting along depth direction as marked above. This curving artefact is used to explain the apparent widening of the oxide layer in the following 1D composition profiles.

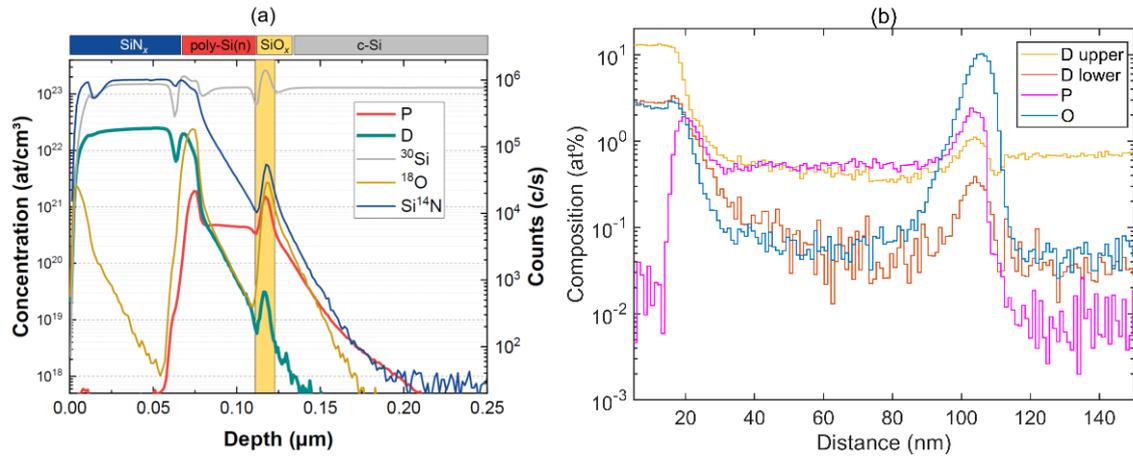


Figure S4. (a) SIMS depths profiles of species in at/cm^3 for an equivalent TOPCon sample, recorded by CAMECA IMS 4fE6. Primary-ion: Cs^+ at 14.5 keV. Si- calibration on implantation standard 2H in Si; P, D are calibrated at at/cm^3 ; Uncalibrated (cont/s): ^{30}Si , ^{18}O , Si^{14}N . (b) APT depths profiles of species in at% replotted on a log scale.

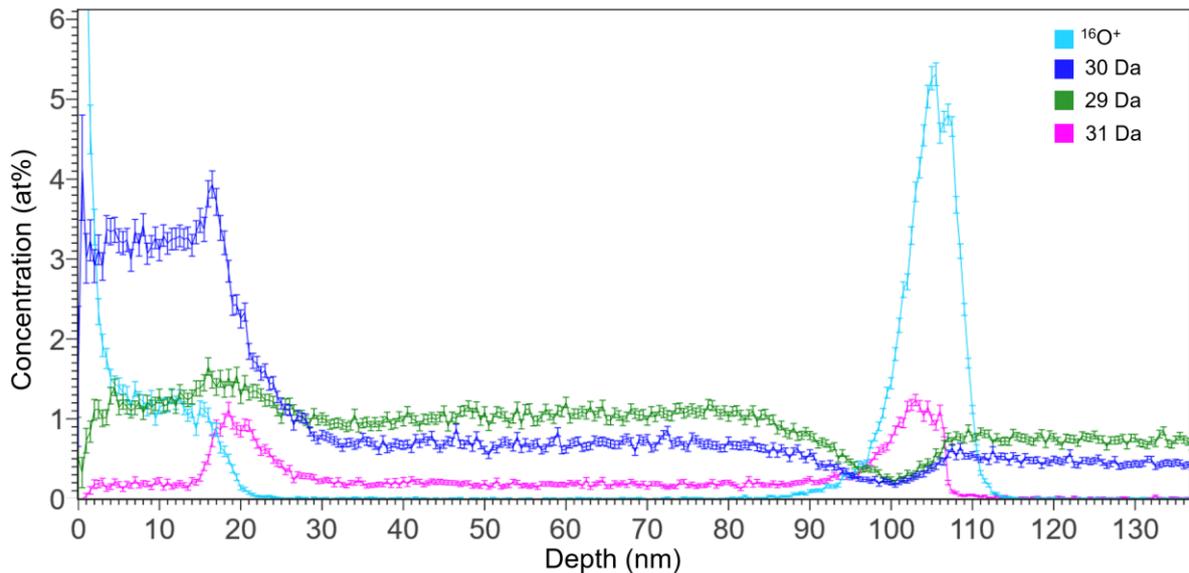


Figure S5. Concentration profiles along depth for ionic species, without overlap solving. Included here $^{16}\text{O}^+$ at 16 Da; $^{28}\text{SiH}^+ / ^{29}\text{Si}^+$ at 29 Da; $^{28}\text{SiD}^+ / ^{29}\text{SiH}^+ / ^{30}\text{Si}^+$ at 30 Da; and $\text{P}^+ / ^{30}\text{SiH}^+ / ^{29}\text{SiD}^+$ at 31 Da

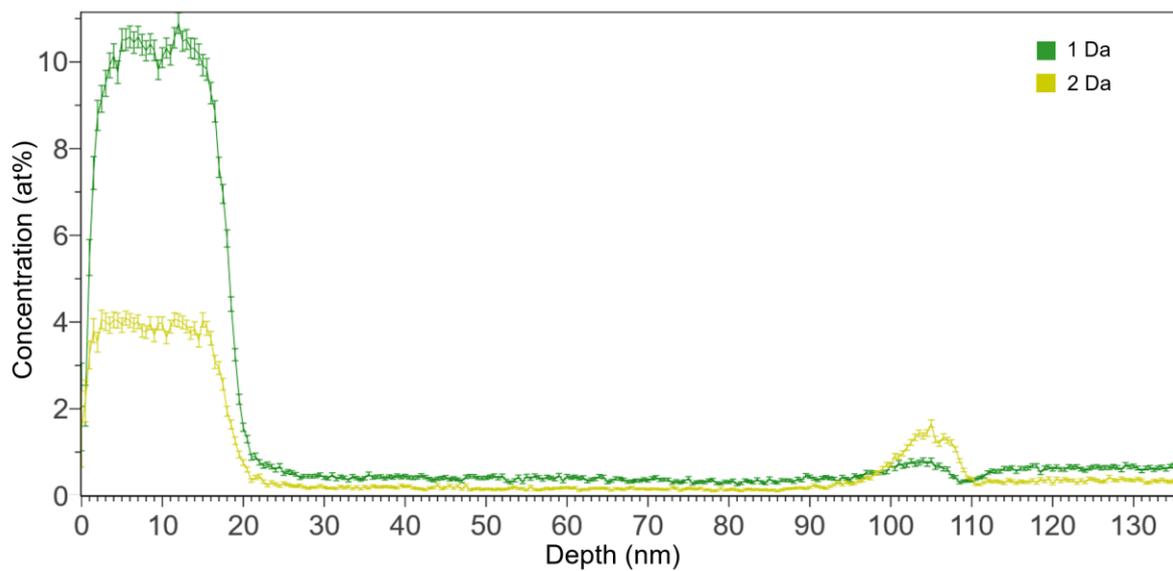


Figure S6. Concentration profiles along depth for ionic species, without overlap solving. Included here: H⁺ at 1 Da; D⁺/H₂⁺ at 2 Da.