QDB: A new database of plasma chemistries and reactions – concept and exemplar verification.

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Quantemol Ltd

Quantemol is based at University College London and was founded by Prof. Jonathan Tennyson FRS and Dr Daniel Brown in 2004. The company develops unique software tools that bring accessibility to highly sophisticated research codes

Research objectives

A key goal of the presented research project PowerBase is to produce new integration schemes which enable the manufacturability of 3D integrated power smart systems with high precision through-silicon via etched features. The necessary high aspect ratio etch is performed via the BOSCH process. Investigations in industrial research often use trial and improvement experimental methods. Simulations provide an alternative way to study the influence of external parameters on the final product, whilst also giving insights into the physical processes.

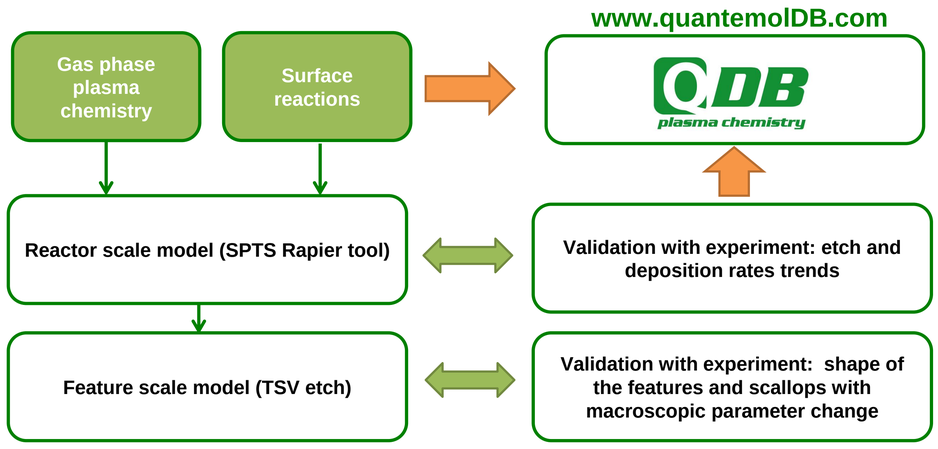


Fig 1. Schematics showing the project work flow and how QDB becomes a distribution channel for Powerbase work where pre-assembled chemistry sets and validation are being deposited.

Data Model

In QDB[1] reactions and chemistries are presented in linked tables in a relational database. This allows users to make searches of the database to retrieve cross section and Arrhenius parameter data with visualization in their browsers. Pre-assembled chemistry sets can be downloaded in one file in a flexible format but also connected via API to Quantemol-VT software tool. This creates a software solution including dynamic chemistry data for complex industrial chemistry sets.

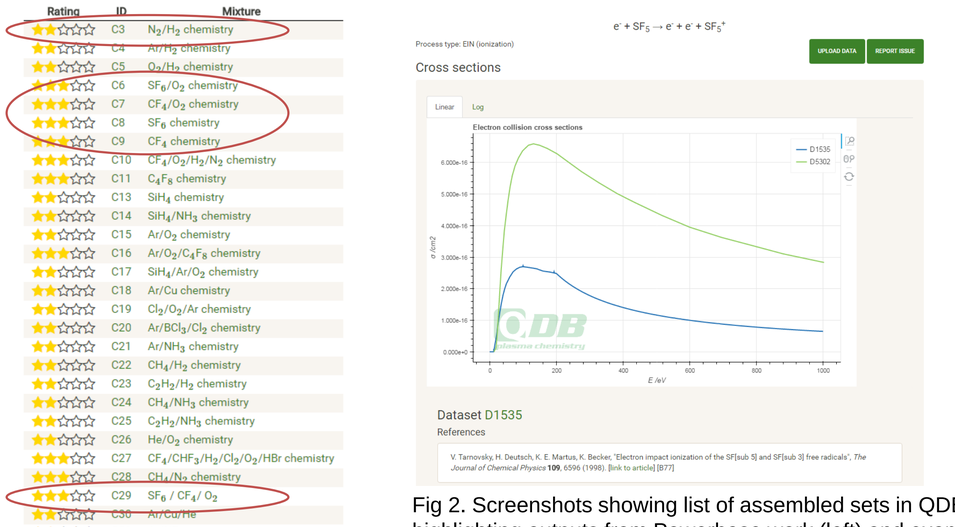


Fig 2. Screenshots showing list of assembled sets in QDB highlighting outputs from Powerbase work (left) and example of individual reactions data representation (above)

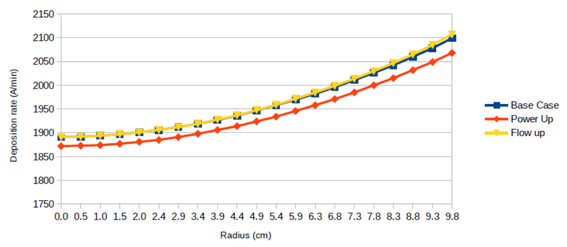
Data sets: 5147
Reaction rates: 2259; Cross sections: 2888
Chemistry sets: 29

[1] Tennyson et al, QDB: a new database of plasma chemistries and reactions, PSST (GEC special issue, 2017) in press.

Effect of Chemistry Variation on Polymer Deposition in a C_4F_8 ICP

As an example for the effect of the chemistry on process relevant parameters, we compare the deposition rate of polymers on a blank silicon wafer in a C_4F_8 discharge, we compare a case with neglected 3-body collision (1) and one with high rate coefficients for these reactions on the order of $10^{-11}cm^3s^{-1}$ when treated as two-body collisions (2).

(1)



(2)

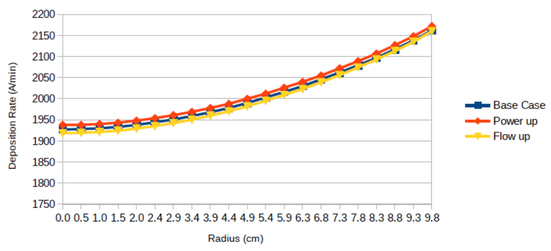


Fig 3. Trends comparing neglected 3-body collisions case (1) one with high rate coefficients for these reactions when treated as two-body collisions (2).

Adding 3-body collisions increases the absolute deposition rate. Furthermore, the trend of the deposition rate as a function of power reverses: without these reactions, it decreases; with 3-body collisions it increases. The flow variation is not affected. Hence, it is really important to include these reactions in the chemistry to understand the kinetics influencing deposition rate.

Current reactor scale validation results

The reactor scale models were developed separately for etch and deposition steps. The validation was performed using experimental data available from the tool manufacturer on blanket wafer etch and deposition. Surface chemistry was constructed for a fixed wafer temperature in both models and pressure, power and flow variations in the models were performed.

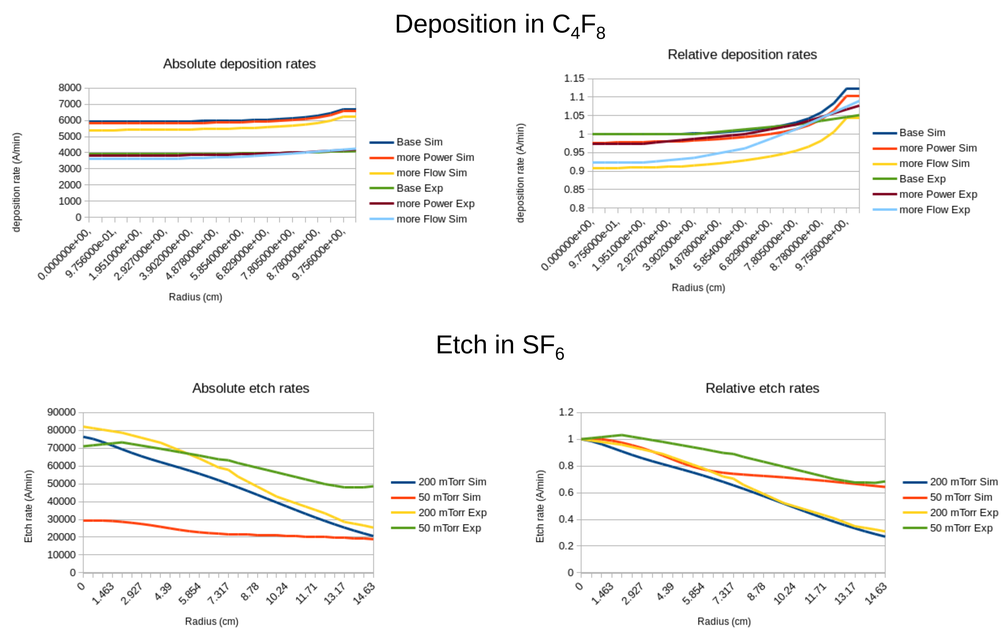
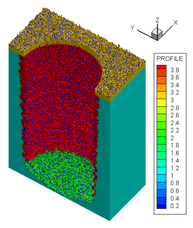


Fig 4. Graphs comparing absolute and relative etch and deposition rates in SPTS Rapier tool for BOSCH process modelling.

In general, good to excellent agreement was achieved. The observed differences can be attributed to uncertainties in pressure-dependent rate coefficients and surface reactions. Experimental results provided by SPTS.

The next step outlook

Current data validated models of etch and deposition steps in the BOSCH process for TSV generate angular and energy distributions on the wafer and then used in a consecutive feature scale modelling of the TSV. A variation of the reactor scale parameters around the process recipe will be used to identify optimum combination. The criteria in choosing an optimum parameter set are: best achievable uniformity over the entire wafer; less scallops (or smoother); layer thickness uniformity over the entire TSV height; rounded corners at bottom.



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