Progress on the construction of software tools designed to help solve the plasma chemistry data problem.

James J Munro[1], Jonathan Tennyson and Natasha Doss

University College London, Gower Street, London, WC1E 6BT, UK

[1]james@theory.phys.ucl.ac.uk

Here we present progress on the construction of a sophisticated global model for plasma processing. Quantemol-P [1] (Q-P) builds upon GlobalKin [2], a non-equilibrium zero-d plasma source model that includes a Boltzmann solver for the electron energy distribution and a stiff ODE solver for the chemical kinetics. Q-P uses cross-section data and a model of plasma chemistries to help automate the process of chemistry generation and simulation. Both existing cross-section data and new cross-section data from Q-P's sister software tool Quantemol-N [3] are used to populate the database.

Quantemol-N calculations for electron-impact excitation and dissociation and are shown for CF2 giving effective cross-sections for the following reactions,

$$\begin{aligned} e + CF_2 &\rightarrow e + CF_2^*(^3B_1) \\ e + CF_2 &\rightarrow e + CF + F \\ e + CF_2^*(^3B_1) &\rightarrow e + CF_2 \\ e + CF_2^*(^3B_1) &\rightarrow e + CF + F. \end{aligned}$$

Q-P calculations are demonstrated for a chemical SF6/O2 plasma-enhanced silicon etch using an inductively coupled plasma source.

[1] J. J. Munro and J. Tennyson, J. Vac. Sci. Tech. A 26, 865 (2008).
[2] D. S. Stafford and M. J. Kushner, J. Appl. Phys. 96, 2451 (2004).
[3] J. Tennyson, D. Brown, J. J. Munro, I. Rozum, H. N. Varambhia and N. Vinci, J. Phys.: Conf. Ser. 86, 012001 (2007).