

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

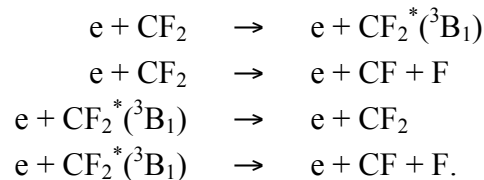
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Here we present progress on the construction of a sophisticated global model for plasma processing. Quantemol-P [1] (Q-P) builds upon GlobalKin [2], a non-equilibrium zero-d plasma source model that includes a Boltzmann solver for the electron energy 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,



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).