QUANTEMOL VALIDATED CHEMISTRY DATABASE: CALCULATED CROSS SECTIONS FOR ELECTRON NF_x COLLISIONS AS AN EXAMPLE

J.R. Hamilton[a,b], S. Huang[c], M. J. Kushner[c], S. Rahimi[b], C. Hill[a], A. Dzarasova[b], and J. Tennyson[a,b]

[a] Dept. of Physics and Astronomy, University College London, London WC1E 6BT, UK
[b]Quantemol Ltd., London, NW3 4HA, UK
[c] Dept. of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor MI 48109-2122, USA

Nitrogen trifluoride (NF_3) is used in a variety of plasma processes incuding direct etching [1,2], reactor cleaning [3] and remote plasma sources (RPS) due to the ease with which F atoms are produced by dissociative attachment. RPS sustained only in NF_3 typically limits the types of reactive fluxes reaching the processing chamber to only F_x and NF_x atoms and molecules. Models of such plasmas are severly limited by the absence of almost any data on the molecules created by the dissociation of NF_3, namely nitrogen diflouride (NF_2) and nitorgen monoflouride (NF). Here we present the conclusions of an investigation into important electron impact processes involving NF_x species using the R-Matrix method and other established theoretical methods. We also present cross sections for processes which cannot be calculated rigirously namely ionisation dissociation and electron impact dissociation breaking up NF_x into specific products using methods developed during this investigation.

One of most challenging recurring problems when modelling plasmas is the scarcity of data. This lack of complete and validated datasets hinders research on plasma processes and slows development of industrial applications [4]. We will present the Quantemol DataBase (QDB) project which aims to fill this missing link by provide a platform for exchange and validation of chemistry datasets. The online database will collate published data on both electron scattering and heavy particle reactions, and so facilitate and encourage peer-to-peer data sharing by its users. This data platform is rigorously supported by the methodical validation of the datasets. An automated Chemistry Generator (CG) is employed which identifies missing reactions in the reaction mechanism which, although important, are currently unreported in the literature. The CG employs mathematical methods to analyze the importance of these chemistries and these gaps in the datasets are filled using theoretical methods.

References

[1] L. Pruette, S. Karecki, R. Chatterjee, R. Reif, T. Sparks, and V. Vartanian, “High density plasma oxide etching using nitrogen trifluoride and acetylene” J. Vac. Sci. Tech. A **18**, 2749-2758 (2000).

[2] J. M. Veilleux, M. S. El-Genk, E. P. Chamberlin, C. Munson, and J. FitzPatrick, “Etching of UO_2 in NF_3 RF plasma glow discharge” J. Nuc. Mat. **277,** 315-324 (2000).

[3] G. Bruno, P. Capezzuto, G. Cicala and P. Manodoro, “Study of the NF_3 plasma cleaning of reactors for amorphous-silicon deposition” J. Vac. Sci. Tech. A **12**, 690-698 (1994).

[4] K. Bartschat and M. J. Kushner, Proc. Nat. Acad. Sci. (2016), in press,