Data needs for industrial plasma processes modelling and optimisation

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Computational simulations of plasmas in both academic and industrial research play an important role for both gaining a better understanding of fundamental plasma processes and improving industrial processes. The validity of such simulations is highly influenced by two factors: the robustness of the physical models and the correct choice of plasma species and reactions. While advances in the former are mostly driven by improving numerical and computational techniques, the latter depends mostly on the availability of reliable data on reactions. While these data such as electron impact cross sections can often be found for feed gases such as argon or CF_4, they are not readily available for species produced in the plasma, for example by dissociation or at surfaces. Furthermore, they cannot be easily measured, so theoretical calculations are often the only means to obtain these important data.

Apart from finding data on individual reactions, the compilation of a fitting set of reactions for a given problem is an important step. While it is tempting to simply use all available reactions, this often results in unnecessarily complicated reaction mechanisms which compromise the speed and stability of the simulations. Furthermore, it complicates the analysis of the results such as the identifying the role of specific species in a given setup. As the importance of individual species and reactions depend highly on the process parameters such as the pressure, a clever design of the plasma chemistry will not only improve the validity of the simulation results, but also the computational speed and robustness.

This presentation will highlight the data needs for specific type of reactions such electron impact collisions, heavy particle collisions, and surface reactions, discuss the influence of uncertainties on the final simulation results, and present solutions to obtain both fundamental data such as cross sections and complete chemistry sets.