# Hydrogen, Helium and Lithium plasmas: from the dynamics of elementary processes to modeling of fusion devices

Wednesday, 7 October 2020 13:30 (30 minutes)

One of the problems arising in thermonuclear fusion research, is represented by the excessive thermal load on plasma facing components of fusion devices, coming from the intense heat flux reaching the material surfaces. A possible strategy, aimed to the reduction of the thermal exposure, is represented by the use of liquid metals, which, after evaporation, leads, through interaction with the main plasma, to the conversion of the thermal energy in radiation, which is finally dispersed in the plasma bulk. This conversion process reduces the heat flux on the reactor walls, generated by the particle impacts, thus preventing the thermal degradation and chemical erosion of the material components. Among the many candidates for vapour shielding, lithium is considered one of the most promising metals.

After evaporation, the lithium atoms present in gas phase, can give rise to reactive processes which can yield to the formation of molecular species, like Li2 dimers or LiH hydrides. These molecules, animated by internal rovibronic motions, can play a non-negligible role in the conversion of internal energy in radiation. A general mechanism for radiative processes involving molecules, is represented by the excitation of the internal states by particle collisions, followed by photon emission. Typical example is given by the so-called radiative decay which can be represented by the following two-step process (also known as E-V process) [1]:

$$M_2(X, \nu) + e \rightarrow M_2(A, \nu'') + e \rightarrow M_2(X, \nu') + e + \hbar\omega \quad (1)$$
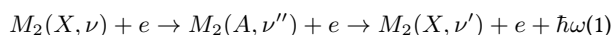
In the first step the diatomic molecule, M_2, in one of the vibrational levels of its ground electronic state, (X, ν), is excited by electron impact to the spectroscopically allowed vibro-electronic state (A, ν''), followed by the decay again in the vibrational manifold of the ground state, included the dissociative continuum, through the emission of a photon with frequency ω. The calculation of the cross section for this process requires the electron-impact cross section data for the first step, as well as the emission Einstein coefficients for the second. Experience acquired with other electron-molecule scattering systems, shows that both these quantities heavily depend on the initial vibrational excitation of the molecule.

A theoretical modeling, aimed to the simulation of the best conditions for an efficient vapour shielding in fusion plasmas, must include, thus, the description of the vibrational kinetic for a realistic determination of the time-dependent vibrational population of all molecular species acting in the plasma. The very first step for the construction of such model, starts from the knowledge of the collision cross sections for vibrational energy exchanges of molecular species with all the other particles present in the system.

In our group, we have started the calculations of electron collision cross sections involving vibrationally excited LiH. In particular, cross sections and rate coefficients have been calculated for the vibro-electronic transition $LiH(X^1\Sigma^+, \nu) + e- > LiH(A^1\Sigma^+, \nu') + e$, by using a modified form of the Mott and Massey scattering approximation [2]. The complete dataset has been derived for the excitations from the 24 vibrational levels of the ground state. The state-to-state cross sections for the $\nu \rightarrow \nu' = \nu$ excitations display a significant increase with the vibrational energy content (see Fig.1), reflecting the behavior of the transition dipole moment with the stretching of the molecular bond. Moreover, analytical functions have been derived that accurately reproduce the energy profile of the cross sections for their easy implementation in kinetic models.

[1] R. Celiberto, M. Capitelli, U. Lamanna, Chemical Physics, 183, 101 (1994).
[2] R. Celiberto, R. K. Janev and A. Laricchiuta, Plasma Sources Sci. Technol., 29, 035008 (2020).

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Session Classification: Fundamental modelling and theories