ELECTRON IONIZATION CROSS SECTIONS FOR ATOMS, MOLECULES AND MOLECULAR IONS RELEVANT TO FUSION EDGE PLASMAS: EXPERIMENT AND THEORY

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1. Introduction

Recent studies in the field of thermonuclear fusion based on the magnetic confinement of high temperature plasmas have demonstrated that the conditions at the plasma periphery („plasma edge") play an important role for achieving, sustaining and controlling thermonuclear fusion plasmas [1]. In order to understand and elucidate the role of radiative and collisional processes in the plasma edge region, in particular their influence on the plasma properties and dynamics and their use for controlling the plasma conditions, it is essential to have available a detailed and quantitative knowledge on these elementary processes. The plasma edge region contains a significant number of a variety of atomic ions, many of which are introduced by impurities from e.g. the protective tiles of the first wall and the divertor plates. Janev [1] has given a comprehensive list of atomic and molecular impurities to be considered in such studies.

The present investigation is concerned with providing quantitative information on electron ionization processes involving various plasma edge constituents, including total, partial and differential ionization cross sections and ionization energies. For this purpose we have developed and extended on the one hand theoretical methods and on the other hand experimental techniques thus allowing us to determine these cross sections and ionization energies with high accuracy. As examples we will present recent results on

(i) calculated cross sections for the formation of highly charged ions by electron ionization of neutral atoms

(ii) calculated electron ionization cross sections of complex molecules

(iii) measured partial electron ionization cross sections for hydrocarbon molecules

(iv) measured kinetic energy release distributions (KERD's) for fragment ions produced via electron ionization of polyatomic molecules at various times after the ionization event (prompt and metastable dissociations)

(v) measured partial ionization cross sections and KERD’s for polyatomic ions, and

(vi) measured ionization energies and attachment cross sections for simple molecules.

2.1. Experimental studies about electron ionization of neutrals and ions

2.1.1. Determination of partial and total cross sections, kinetic energy releases and ionization energies:

The experimental crossed-beams sector-field mass-spectrometer (CSM) set-up and the procedure used in our laboratory for the accurate measurement of partial ionization cross sections of atoms and of molecules consists of a modified Nier-type electron impact ion source, a molecular beam source (either a Knudsen-type oven or a nozzle expansion source) and a high resolution double focussing two-sector field mass spectrometer. The performance and operating conditions of this apparatus have been continuously improved over the past 15 years. Today it is possible to measure (absolute) partial ionization cross section functions for atomic and molecular parent ions as well as partial ionization cross section functions for fragment ions formed with excess kinetic energy with high accuracy up to electron energies of 1000 eV. As shown in these studies it is (i) necessary (in order to account quantitatively for discrimination effects in the case of fragment ions produced with excess kinetic energy in the ion source) and it is (ii) also possible to measure the kinetic energy release distributions (KERD) of the fragment ions formed by electron impact ionization either in the ion source (prompt decay) or at a later times (metastable decay). In order to study the prompt fragmentations we have developed over the years in our laboratory the ion beam deflection, IBD, method (based on the fact that the extracted ion beam shape contains information on the original ion kinetic distribution of the ions produced by electron ionization of the neutral targets) and in addition recently a new method (mass analyzed redarding potential, MARP, method) using the tandem mass-spectrometer apparatus BESTOF described in Ref. [1]. Moreover, to study the metastable decay reactions in the second field free region we have improved the well known MIKE scan method. Using all three methods we have studied in detail KED’s, KERD’s and the average total kinetic energy release (<KER>) deduced from these distributions for C_3H_8 and are presently in addition starting with measurements of further small hydrocarbons (see also Ref. [2-4].

Moreover, using monochromatized electrons (from a hemispherical electron monochromator, HEM) in a newly constructed high resolution crossed-beams/quadrupole mass spectrometer (CQM) apparatus we were able to (i) measure in great detail the ionization threshold region and thus to (ii) deduce ionization energies; first examples of this include ionization energies of CO, $(CO)_2$ and $(CO)_3$ [5].

In addition, as high current H^- ion sources are of potential interest in future fusion reactors we have also started high resolution electron attachment studies with a recently constructed high resolution trochoidal electron monochromator (TEM) apparatus (supported by studies with the HEM) including investigations for NO, CO and CO_2 (see also Ref. [6-8].

2.1.2. Electron impact ionization/dissociation of mass selected molecular ions

In order to study electron induced ionization and dissociation of mass selected molecular ions, we have recently modified the two sector field mass spectrometer system (CSM) in such a way as to allow with help of a newly constructed high performance electrun gun the study of inelastic interactions between electrons and ions in the ion beam focus of the second field free region (half way between the magnetic and the electrostatic field). After first tests with this method we have studied the ionization of propane ions as a first prototypical case and obtained first results on the KERD and <KER> values for several decay reactions induced by electron impact on mass selected propane or propane fragment ions [4].

2.2. Theoretical studies about electron ionization of neutrals and ions

Scaling laws and semiempirical methods can be powerfool tools to predict electron impact ionization cross sections for neutrals and ions for modelling purposes in particular for those targets where experimental data do not exist and/or rigorous theoretical calculations are inconvenient or impossible. Because classical, semi-classical and semi-empirical formulae fail in certain even simple cases, we have suggested in 1987 [9] the use of a semi-classical approach based on a combination of the binary encounter approximation and the Born-Bethe approximation. In the frame of the Euratom-ÖAW association we have started to apply this DM concept [10] to fusion relevant cases, including here innershell ionization and multiple ionization [11,12].

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