

Electron Impact Ionization and Surface Induced Reactions of Fusion Plasma Edge Constituents

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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 the thermonuclear fusion plasma [1]. In order to understand and elucidate the role of the 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 such as cross sections, reaction rate coefficients etc. Because of the relatively low temperature in the plasma edge the plasma contains - besides electrons and atomic ions - also a significant number of neutral hydrogen atoms, low-charged atomic and molecular impurities (produced and introduced for instance via plasma/wall interactions [2], via diagnostics or via cooling). According to Janev [1] the most important collision processes (from a standpoint of their effects on plasma edge properties and behavior such as ionization balance, plasma energy, plasma transport etc.) are electron impact excitation/ionization reactions with plasma edge atoms, ions and molecules [3-5]. The impurities present in such an edge plasma obviously will depend on the materials used for the plasma facing components (first wall, protective tiles, divertor plates, antennas for rf heating etc.) and on the gases introduced for cooling and diagnostic purposes. Janev [1] has given a list of atomic and molecular impurities to be considered in such studies including the rare gases, Li, Be, B, C, Al, Si, Mg, Ti, Cr, Fe, Ni, Cu, Mo, Nb, Ta, W, and CO, CO₂, CH₄, C₂H₂, C_nH_m, H₂O. Some of these impurities may reach levels of about 1 to several percent of the plasma density.

Whereas electron impact ionization of neutral and ionized *atomic* targets is a well studied and documented subject [3,4] (save for a few targets and for some cases involving multiple and step-wise ionization), the situation in case of *molecular* targets is far from satisfying. According to Tawara [5], who reviewed electron impact ionization of hydrocarbon molecules many data (concerning total and partial ionization cross sections) appear to be of relatively low accuracy or have not yet been measured. The latter applies in particular to hydrocarbon molecular ions, where almost no experimental (and theoretical) studies exist (see also Ref [6]). Moreover, the subject of electron impact induced ionization of molecular ions has so far received very little attention (in contrast to the field of electron impact ionization of atomic ions [7]). A similar situation exists for the area of plasma/wall interactions [2], where an understanding of the individual "surface erosion processes" for the various target materials, in particular under typical reactor edge plasma conditions, is a crucial prerequisite for designing the thermonuclear fusion reactor.

The present long term data study is dedicated to provide this *quantitative information* for the various plasma edge constituents including, (i) experimental and theoretical studies about the ionization of neutrals and ions, and (ii) reactive interaction of molecular ions with surfaces. The present studies constitute on the one hand a continuation of previous research in our laboratories (i.e., on the experimental determination of accurate ionization cross sections for neutral molecules and on theoretical concepts for the prediction of ionization cross sections for various targets, i.e., atoms, molecules and clusters [8]) and on the other hand an extension of recently started experiments on the inelastic interaction of electrons with molecular ions [9] and on reactive scattering of molecular ions on surfaces. These previous studies (and the available techniques) and also these preliminary and exploratory studies will be summarized and based on this background an outline of the present research will be given.

2 Electron Impact Ionization of Neutral Molecules: Experimental Determination of Cross Section, Kinetic Energy Release and Ionization Energy

A detailed description of the apparatus and the experimental procedure used in our laboratory for the accurate measurement of partial ionization cross sections of atoms and of molecules has been given previously [10]. Briefly, the experimental set-up 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 Nier-Johnson 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 [10]. This was tested recently in detail with CF_4 [10] and used recently for the study of C_2H_6 [11], C_3H_8 [12] and C_{60} [13].

As shown and discussed in [10] it is 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 possible to measure the kinetic energy release distributions (KERD) of the fragment ions formed by electron impact ionization in the ion source using a method developed over the years in our laboratory. This ion beam deflection method is based on the fact that the extracted ion beam shape contains information on the original ion kinetic distribution [10-12]. Detailed studies about KERDs and the average total kinetic energy release (KER) deduced from these distributions have been performed recently for C_3H_8 [14] and C_{60} [15] and are presently also carried out employing a new experimental method using the apparatus described in section 5.

Moreover, using monochromatized electrons in a newly constructed high resolution ion source/mass spectrometer 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 singly- and multiply-charged parent [16] and fragment [17] fullerene ions and ionization energies of CO clusters [18].

3 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 [19] our two-sector-field mass spectrometer system in such a way as to allow with help of a newly constructed high performance electron 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). Ions passing this second field free region have already been mass selected by the magnetic sector field. Because ions are produced in this set-up by an ordinary electron-impact ionization Nier type ion source, the primary ion currents available after mass selection are in the order of about 10 pA. With the present electron gun (with electron currents of about 10 mA) mounted between the two sectors it became possible to investigate electron induced ionization and fragmentation of mass selected ions. In particular we used the MIKE-scan (mass analysed ion kinetic energy scan) technique [20] (which can be used also to study the spontaneous decay of molecular ions in the metastable time regime) in order to identify and analyse fragment ions in terms of their mass and charge state and their kinetic energy release. The position of the respective MIKE peaks allows an unambiguous identification of the parent and fragment ion peaks produced and from the shape of a MIKE peak it is possible to derive the total kinetic energy release distribution (KERD) of a specific decay reaction. In a further step the average total kinetic energy release (KER value) of the decay reaction can be determined by calculating the first momentum of the KERD. So far we have used this technique to study the properties of singly- and multiply-charged fullerene ions [19].

4 Calculation of Ionization Cross Sections for Multiple Ionization of Atoms and Atomic Ions

Scaling laws and semiempirical methods can be powerful 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. Many practical applications require either a quick estimate of a large number of ionization cross sections or ionization cross section functions in analytical form [21]. Such needs can often be satisfied best (i.e., most economically and least time consuming to the practitioner) through the use of scaling laws and other simple methods. Because classical, semi-classical and semi-empirical formulae fail in certain even simple cases [22], we have suggested in 1987 [23] the use of a semi-classical approach based on a combination of the binary encounter approximation and the Born-Bethe approximation. Although originally devised for the single ionization of ground state atoms [22,23], this concept has been successfully extended to the single ionization of excited atoms, free radicals, molecules, clusters and fullerenes and atomic ions and to the ionization of specific shells of atoms (for more details see accompanying paper in this conference). Very recently, we have also started to apply this concept to the case of multiple ionization of atoms, so far including double and triple ionization [24] and quadruple and quintuple ionization [25], and very recently even to charge states higher than 5 of neutral atoms [26].

5 Reactive Interactions of Molecular Ions with Surfaces

Recently we have constructed in our laboratory a new tandem mass spectrometer [27] consisting of an ion source, a two sector field mass spectrometer, deceleration ion optics, a surface collision chamber and a time of flight mass spectrometer. This apparatus allows us to study the various surface induced reactions such as surface induced dissociation, ion surface reactions and chemical sputtering as a function of collision energy (from threshold up to about 3 kV). Thus we are able to obtain information about the mechanisms, the kinetics and the energetics of the reactions occurring. After first tests we have so far studied reactions of acetone and benzene ions and their respective cluster ions [27-30], fullerene ions and various other fusion relevant ions with hydrocarbon covered stainless steel surfaces.

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